



# STIC Search Report

## Biotech-Chem Library

STIC Database Tracking Number: 127375

TO: Hector Reyes  
Location: REM-5C18  
Art Unit: 1625  
Wednesday, July 21, 2004

Case Serial Number: 10/075442

From: Deirdre Arnold  
Location: Biotech-Chem Library  
REM 1A64  
Phone: 571-272-2532

Deirdre.Arnold@uspto.gov

### Search Notes

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# STIC SEARCH RESULT FEEDBACK FORM

## Biotech-Chem Library

Questions about the scope or the results of the search? Contact *the searcher* or contact

Mary Hale, Information Branch Supervisor  
571-272-2507 Remsen E01 D86

## Voluntary Results Feedback Form

➤ I am an examiner in Workgroup:  Example: 1610

➤ Relevant prior art **found**, search results used as follows:

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature  
(journal articles, conference proceedings, new product announcements etc.)

➤ Relevant prior art **not found**:

- ☐ Results verified the lack of relevant prior art (helped determine patentability)
- ☐ Results were not useful in determining patentability or understanding the invention

Comments:

Drop off or send completed forms to STIC/Biotech-Chem Library Remsen Bldg



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FILE COVERS 1907 - 21 Jul 2004 VOL 141 ISS 4  
 FILE LAST UPDATED: 20 Jul 2004 (20040720/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> act rey442hcaapp/a

L24 1 SEA FILE=HCAPLUS ABB=ON PLU=ON US2002-075442/AP,PRN

=> d que l24

L24 1 SEA FILE=HCAPLUS ABB=ON PLU=ON US2002-075442/AP,PRN

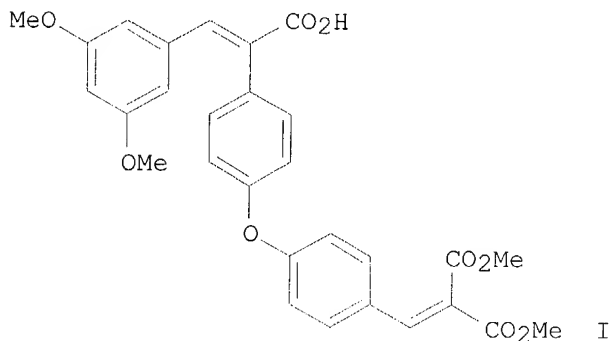
=> d l24 iall

L24 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2001:359750 HCAPLUS  
 DOCUMENT NUMBER: 134:348284  
 ENTRY DATE: Entered STN: 18 May 2001  
 TITLE: Phenyl compounds to treat diabetes and associated conditions  
 INVENTOR(S): Neogi, Partha; Nag, Bishwajit; Lakner, Frederick J.;  
 DeY, Debendranath; Medicherla, Satyanarayana  
 PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA  
 SOURCE: PCT Int. Appl., 47 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 INT. PATENT CLASSIF.:  
 MAIN: A61K  
 CLASSIFICATION: 1-10 (Pharmacology)  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001034094	A2	20010517	WO 2000-US30927	20001108
WO 2001034094	C2	20020725		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,  
 CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,  
 HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,

LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,  
 SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,  
 YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
 US 6525093 B1 20030225 US 1999-436047 19991108  
 AU 2001017607 A5 20010606 AU 2001-17607 20001108  
 EP 1235785 A2 20020904 EP 2000-980331 20001108  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
 JP 2004503464 T2 20040205 JP 2001-536099 20001108  
 US 2002107285 A1 20020808 US 2002-75442 20020215 <--  
 PRIORITY APPLN. INFO.: US 1999-436047 A 19991108  
 WO 2000-US30927 W 20001108  
 OTHER SOURCE(S): MARPAT 134:348284  
 GRAPHIC IMAGE:



## ABSTRACT:

Ph compds. (Markush included) are provided that lower blood glucose concns., lower serum triglyceride concns., lower systolic blood pressure, and increase glucose uptake by adipose tissue, but do not affect the expression of PPAR- $\gamma$  by adipose tissue. Compds. of the invention include e.g. I.

SUPPL. TERM: phenyl deriv antidiabetic hypotriglyceridemic  
 antihypertensive  
 INDEX TERM: Antidiabetic agents  
 Antihypertensives  
 Drug delivery systems  
 Hypolipemic agents  
 (Ph compds. to treat diabetes and associated conditions)  
 INDEX TERM: Glycerides, biological studies  
 ROLE: BPR (Biological process); BSU (Biological study,  
 unclassified); BIOL (Biological study); PROC (Process)  
 (blood; Ph compds. to treat diabetes and associated  
 conditions)  
 INDEX TERM: Peroxisome proliferator-activated receptors  
 ROLE: BPR (Biological process); BSU (Biological study,  
 unclassified); BIOL (Biological study); PROC (Process)  
 ( $\gamma$ ; Ph compds. to treat diabetes and associated  
 conditions)  
 INDEX TERM: 339332-56-8 339332-57-9  
 ROLE: BAC (Biological activity or effector, except adverse);

BSU (Biological study, unclassified); THU (Therapeutic use);  
BIOL (Biological study); USES (Uses)  
INDEX TERM: (Ph compds. to treat diabetes and associated conditions)  
50-99-7, D-Glucose, biological studies  
ROLE: BPR (Biological process); BSU (Biological study,  
unclassified); BIOL (Biological study); PROC (Process)  
(Ph compds. to treat diabetes and associated conditions)

=> FIL STNGUIDE

=> fil zcaplus

FILE 'ZCAPLUS' ENTERED AT 08:36:01 ON 21 JUL 2004  
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FILE COVERS 1907 - 21 Jul 2004 VOL 141 ISS 4  
FILE LAST UPDATED: 20 Jul 2004 (20040720/ED)

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=> fil hcaplus

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=> fil biosis

FILE 'BIOSIS' ENTERED AT 08:36:06 ON 21 JUL 2004  
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FILE COVERS 1969 TO DATE.  
CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNS) PRESENT  
FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 15 July 2004 (20040715/ED)

FILE RELOADED: 19 October 2003.

=> FIL STNGUIDE

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FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Jul 16, 2004 (20040716/UP).

=> d que l10

L1 ( 114)SEA FILE=HCAPLUS ABB=ON PLU=ON ("NEOGI P"/AU OR "NEOGI P K  
B"/AU OR "NEOGI P S"/AU) OR ("NEOGI PARTHA"/AU OR "NEOGI  
PARTHASAKHA"/AU)  
L2 ( 287)SEA FILE=HCAPLUS ABB=ON PLU=ON NAG/AU OR ("NAG B"/AU OR "NAG  
B B"/AU OR "NAG B B S P"/AU OR "NAG B D"/AU OR "NAG B D  
CHOWDHURI"/AU OR "NAG B L"/AU OR "NAG B N"/AU OR "NAG B R"/AU)  
OR ("NAG BISHWAGIT"/AU OR "NAG BISHWAJIT"/AU)  
L3 ( 17)SEA FILE=HCAPLUS ABB=ON PLU=ON ("LAKNER F J"/AU OR "LAKNER  
FREDERICK J"/AU OR "LAKNER FREDERICK JAMES"/AU OR "LAKNER  
FREDRICK J"/AU)  
L4 ( 21)SEA FILE=HCAPLUS ABB=ON PLU=ON ("DEV D"/AU OR "DEV D K"/AU  
OR "DEV D S"/AU OR "DEV D V"/AU) OR "DEV DEBAPRASAD"/AU  
L5 ( 24)SEA FILE=HCAPLUS ABB=ON PLU=ON "MEDICHERIA SATYANARAYANA"/AU  
OR ("MEDICHERLA SATYA"/AU OR "MEDICHERLA SATYANANYANA"/AU OR  
"MEDICHERLA SATYANARAYANA"/AU)  
L6 ( 433)SEA FILE=HCAPLUS ABB=ON PLU=ON (L1 OR L2 OR L3 OR L4 OR L5)  
L7 ( 419)SEA FILE=HCAPLUS ABB=ON PLU=ON L6 AND (AY<2003 OR PY<2003 OR  
PRY<2003)  
L8 ( 22)SEA FILE=HCAPLUS ABB=ON PLU=ON L7 AND ?DIABET?  
L9 ( 11)SEA FILE=HCAPLUS ABB=ON PLU=ON L7 AND ?GLYCERID?  
L10 11 SEA FILE=HCAPLUS ABB=ON PLU=ON L8 AND L9

=> d que l22

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"NAG BISWAJIT"/AU)  
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FRDERICK J"/AU OR "LAKNER FREDERICK J"/AU OR "LAKNER FREDRICK  
J"/AU)  
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"DEV D K"/AU OR "DEV D S"/AU OR "DEV D V"/AU)  
L15 ( 33)SEA FILE=BIOSIS ABB=ON PLU=ON "MEDICHERIA SATYA"/AU OR  
("MEDICHERLA S"/AU OR "MEDICHERLA SATYA"/AU OR "MEDICHERLA  
SATYANANYANA"/AU OR "MEDICHERLA SATYANARAYANA"/AU)  
L16 ( 220)SEA FILE=BIOSIS ABB=ON PLU=ON (L11 OR L12 OR L13 OR L14 OR  
L15)  
L17 ( 11)SEA FILE=BIOSIS ABB=ON PLU=ON L16 AND ?GLYCERID?  
L18 ( 148)SEA FILE=BIOSIS ABB=ON PLU=ON L16 AND (CONG? OR CONF? OR  
SYMP? OR MEET? OR MTG OR FORUM OR FORA OR ASSEM? OR WORK? OR  
WKSHP? OR COLLOQ? OR SESS? OR SEM? OR TRANS? OR PROC? OR ABS?  
OR REV?)/DT,SO,ST,CT,CW,IT,MT,BI  
L19 ( 84)SEA FILE=BIOSIS ABB=ON PLU=ON L16 AND 00520/CC  
L20 ( 85)SEA FILE=BIOSIS ABB=ON PLU=ON (L18 OR L19) NOT ARTICLE/DT

L21 ( 7)SEA FILE=BIOSIS ABB=ON PLU=ON L20 AND ?GLYCER?  
L22 11 SEA FILE=BIOSIS ABB=ON PLU=ON L17 OR L21

=> dup rem l10 l22

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PROCESSING COMPLETED FOR L10  
PROCESSING COMPLETED FOR L22  
L23 20 DUP REM L10 L22 (2 DUPLICATES REMOVED)  
ANSWERS '1-11' FROM FILE HCAPLUS  
ANSWERS '12-20' FROM FILE BIOSIS

=> d ibib abs

L23 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 1  
ACCESSION NUMBER: 2003:747894 HCAPLUS  
DOCUMENT NUMBER: 139.255379  
TITLE: Diphenylethylene compounds for the treatment of  
diabetes  
INVENTOR(S): Nag, Bishwajit; Medicherla,  
Satyanarayana; Dey, Debendranath  
PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA  
SOURCE: U.S., 14 pp., Cont.-in-part of U.S. 6,245,814.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 9  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6624197	B1	20030923	US 2000-642618	20000817 <--
US 6245814	B1	20010612	US 1998-74925	19980508 <--
WO 2001056382	A1	20010809	WO 2001-US3797	20010205 <--
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 2002002200	A1	20020103	US 2001-777551	20010205 <--
EP 1251738	A1	20021030	EP 2001-905454	20010205 <--
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2003521500	T2	20030715	JP 2001-556090	20010205 <--
PRIORITY APPLN. INFO.:			US 1998-74925	A2 19980508 <--
			US 2000-180340P	P 20000204 <--
			US 2000-642618	A 20000817 <--
			WO 2001-US3797	W 20010205 <--
OTHER SOURCE(S):	MARPAT 139:255379			



AB Diphenylethylene and styrene compds. are provided which are administered orally to decrease blood glucose levels in rats. The glucose tolerance in insulin-resistant rats is also shown, as well as lowering of **triglyceride** levels in serum insulin-resistant, hyperinsulinemic and **hypertriglyceridemic** rats. The compds. are orally effective **antidiabetic** agents that potentially may reduce abnormality of glucose and lipid metabolism in **diabetes**. Preparation of 2-(4-hydroxyphenyl)-3-(3,5-dimethoxyphenyl)propenoic acid isomers and sodium salts is described.

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs 2-

YOU HAVE REQUESTED DATA FROM 19 ANSWERS - CONTINUE? Y/(N):y

L23 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2001:627250 HCAPLUS

DOCUMENT NUMBER: 135:162510

TITLE: Diphenylethylene and styrene compounds for the treatment of **diabetes**

INVENTOR(S): **Nag, Bishwajit; Medicherla, Satyanarayana;** Dey, Debendranath

PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA

SOURCE: U.S., 9 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 9

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6245814	B1	20010612	US 1998-74925	19980508 <--
WO 9958127	A1	19991118	WO 1999-US9982	19990507 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9939741	A1	19991129	AU 1999-39741	19990507 <--
AU 751235	B2	20020808		
EP 1007039	A1	20000614	EP 1999-922836	19990507 <--
EP 1007039	B1	20040303		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002514598	T2	20020521	JP 2000-547978	19990507 <--
AT 260906	E	20040315	AT 1999-922836	19990507 <--
NZ 511065	A	20030829	NZ 1999-511065	19990518 <--
US 6624197	B1	20030923	US 2000-642618	20000817 <--
US 2002025975	A1	20020228	US 2001-785554	20010220 <--
US 2002032225	A1	20020314	US 2001-843167	20010427 <--
PRIORITY APPLN. INFO.:			US 1998-74925 A	19980508 <--
			US 1999-287237 A	19990406 <--
			WO 1999-US9982 W	19990507 <--
			US 2000-591105 A2	20000609 <--
			US 2001-785554 A2	20010220 <--

OTHER SOURCE(S): MARPAT 135:162510  
AB Novel diphenylethylene and styrenes are provided which are administered orally to decrease blood glucose levels in rats. The glucose tolerance in insulin resistant rats is also shown, as well as lowering of **triglyceride** levels in serum insulin resistant, hyperinsulinemic and hypertriglycedemic rats. The compds. are orally effective anti-**diabetic** agents that potentially may reduce abnormality of glucose and lipid metabolism in **diabetes**.  
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2003:757334 HCAPLUS  
DOCUMENT NUMBER: 139:276885  
TITLE: Preparation of novel heterocyclic analogs of diphenylethylene compounds as **antidiabetics**  
INVENTOR(S): **Neogi, Partha**; Dey, Debendranath; **Medicherla, Satyanarayana, Nag, Bishwajit**; Lee, Arthur  
PATENT ASSIGNEE(S): USA  
SOURCE: U.S. Pat. Appl. Publ., 66 pp., Cont.-in-part of U.S. Ser. No. 843,167.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 9  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003181494	A1	20030925	US 2002-265902	20021008 <--
US 2002025975	A1	20020228	US 2001-785554	20010220 <--
US 2002032225	A1	20020314	US 2001-843167	20010427 <--
WO 2004033438	A1	20040422	WO 2003-US31803	20031008 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:  
US 1999-287237 A2 19990406 <--  
US 2000-591105 B2 20000609 <--  
US 2001-785554 A2 20010220 <--  
US 2001-843167 A2 20010427 <--  
US 1998-74925 A2 19980508 <--  
US 2002-265902 A2 20021008 <--

OTHER SOURCE(S): MARPAT 139:276885  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compds. [I; Z = II-IV; n, m, q and r = 0-4 (n+m ≤ 4 and

q+r ≤ 4); p, s = 0-5 (p+s ≤ 5); R, R2 = H, alkyl, alkenyl, etc.; R1 = H, alkyl, alkenyl, etc.; A, A1, A2 = H, acylamino, acyloxy, alkanoyl, etc.; B, B1, B2 = H, acylamino, acyloxy, alkanoyl, etc.; or A and B together, or A1 and B1 together, or A2 and B2 together, may be joined to form a methylenedioxy or ethylenedioxy; X, X1 = (un)substituted NH, O, S] which are effective in lowering blood glucose level, serum insulin, **triglyceride** and free fatty acid levels in animal models of Type II **diabetes**, were prepared. E.g., a multi-step synthesis of V, starting from 3,5-dimethoxybenzaldehyde and 4-hydroxyphenylacetic acid, was given. The compound V showed strong glucose lowering activity even though it is a weak PPAR-γ agonist (data given). The compds. I are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis. Pharmaceutical composition comprising the compound I was claimed.

L23 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:185699 HCAPLUS

DOCUMENT NUMBER: 136:247571

TITLE: Preparation of novel heterocyclic analogs of diphenylethylene compounds as inhibitors of cytokines or cyclooxygenase

INVENTOR(S): **Nag, Bishwajit**; Dey, Debendranath;  
**Medicherla, Satyanarayana**; **Neogi, Partha**

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 34 pp., Cont.-in-part of U.S. Ser. No. 785,554.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 9

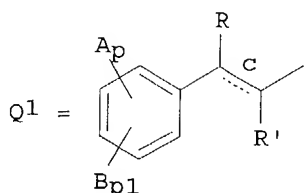
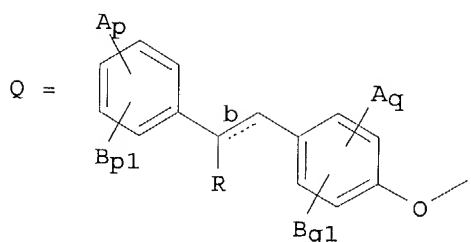
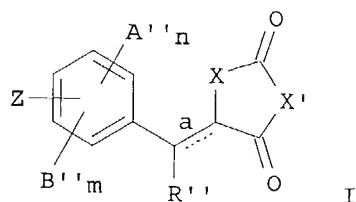
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002032225	A1	20020314	US 2001-843167	20010427 <--
US 6245814	B1	20010612	US 1998-74925	19980508 <--
US 2002025975	A1	20020228	US 2001-785554	20010220 <--
WO 2001095859	A2	20011220	WO 2001-US17950	20010605 <--
WO 2001095859	A3	20030828		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001066670	A5	20011224	AU 2001-66670	20010605 <--
EP 1360178	A2	20031112	EP 2001-944241	20010605 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
US 2003181494	A1	20030925	US 2002-265902	20021008 <--
PRIORITY APPLN. INFO.:				
			US 1998-74925	A2 19980508 <--
			US 1999-287237	A2 19990406 <--
			US 2000-591105	A2 20000609 <--
			US 2001-785554	A2 20010220 <--

US 2001-843167 A2 20010427 <--  
 WO 2001-US17950 W 20010605 <--

OTHER SOURCE(S):  
 GI

MARPAT 136:247571



AB Novel diphenylethylene compds. and derivs. thereof containing thiazolidinedione or oxazolidinedione moieties are provided which are effective in lowering blood glucose level, serum insulin, **triglyceride** and free fatty acid levels in animal models of Type II **diabetes**. The above compds. and their derivs. are resented by formula [I; Z = Q, Q1, H, A'', B''; wherein n, m, q, q1 = integers from zero to 4 provided that  $n+m \leq 4$  and  $q+q1 \leq 4$ ; p, p1 = integers from zero to 5 provided that  $p+p1 \leq 5$ ; a, b and c are double bonds which may be present or absent; when present; the double bonds may be in the E or Z configuration and, when absent, the resulting stereocenters may have the R- or S- configuration; R, R', R'' = H, C1-20 linear or branched alkyl, C2-20 linear or branched alkenyl, CO2Z' (wherein Z' = H, Na, K, or other pharmaceutically acceptable counterion such as Ca, Mg, ammonium, tromethamine, and the like), CO2R'', NH2, NHR'', N(R'')2, OH, OR'', halo, substituted C1-20 linear or branched alkyl or substituted C2-20 linear or branched alkenyl (wherein R'' is C1-20 linear or branched alkyl or linear or branched alkenyl); A, A', A'' = H, C1-20 acylamino, C1-20 acyloxy, C1-20 alkanoyl, C1-20 alkoxycarbonyl, C1-20 alkoxy, C1-20 alkylamino, C1-20 alkylcarboxylamino, CO2H, cyano, halo, HO; B, B', B'' = H, C1-20 acylamino, C1-20 acyloxy, C1-20 alkanoyl, C1-20 alkenoyl, C1-20 alkoxycarbonyl, C1-20 alkoxy, C1-20 alkylamino, C1-20 alkylcarboxylamino, aroyl, aralkanoyl, CO2H, cyano, halo, HO; or A and B together, or A' and B' together, or A'' and B'' together, may be joined to form a methylenedioxy or ethylenedioxy group; and X, X' are independently -NH, -NR'', O or S]. In contrast to previously reported thiazolidinedione compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity. They inhibit the activity of TNF-alpha, interleukin IL-1 or IL-6 or cyclooxygenase-2 (COX-2). The compds. are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis. Thus, To a mixture of 3,5-dimethoxybenzaldehyde (500 g) and

p-hydroxyphenylacetic acid (457 g) was added acetic anhydride (1 L) and triethylamine (420 mL) and the nonhomogeneous mixture on heating became homogeneous at 70° and stirred at 130-140° for 6 h to give 47% 3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid (II) (428 g). II (427.5 g) was suspended in 3 L methanol, treated with 100 mL concentrated H<sub>2</sub>SO<sub>4</sub>, and heated at reflux for 20 h under Ar to give 97% 3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid Me ester (III). III (433 g) was dissolved in 1.6 L DMF, treated with 60.4 g NaH (50% in oil) and the with 185 mL p-fluorobenzaldehyde, and heated at 180° for 18 h to give 77% 3-(3,5-dimethoxyphenyl)-2-[4-(4-formylphenoxy)phenyl]acrylic acid Me ester which (352 g), 2,4-thiazolidinedione 98.6, benzoic acid 134, and piperidine 107.4 g were heated in 2.5 L toluene at reflux with continuous removal of H<sub>2</sub>O through Dean-Stark apparatus to give 86% 3-(3,5-dimethoxyphenyl)-2-[4-[4-(2,4-dioxothiazolidin-5-ylidenemethyl)phenoxy]phenyl]acrylic acid Me ester (IV). IV (30 g) was hydrogenated over 15 g 10% Pd-C in 900 mL dioxane in a Parr apparatus at 60 Psi for 24 h, followed by adding 15 g 10% Pd-C and continuing the hydrogenation for another 24 h to give 86% 3-(3,5-dimethoxyphenyl)-2-[4-[4-(2,4-dioxothiazolidin-5-ylmethyl)phenoxy]phenyl]acrylic acid Me ester (V). When V was orally administered to ob/ob mice with a single oral dose (50 mg/kg body weight), there was a 62 % drop in blood glucose level and, similar to db/db mice, there was no significant increase in body weight between the control and the treatment groups. This was in contrast to treatment of **diabetic** animals by thiazolidinedione type compds. which are known to be associated with increase in body weight

L23 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:158391 HCAPLUS

DOCUMENT NUMBER: 136:216745

TITLE: Preparation and activity of diphenylethylene thiazolidinediones and analogs as **antidiabetics**, antiinflammatories, or immunomodulators

INVENTOR(S): **Nag, Bishwajit**; Dey, Debendranath; **Medicherla, Satyanarayana**; **Neogi, Partha**

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 30 pp., Cont.-in-part of U.S. Ser. No. 591,105.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 9

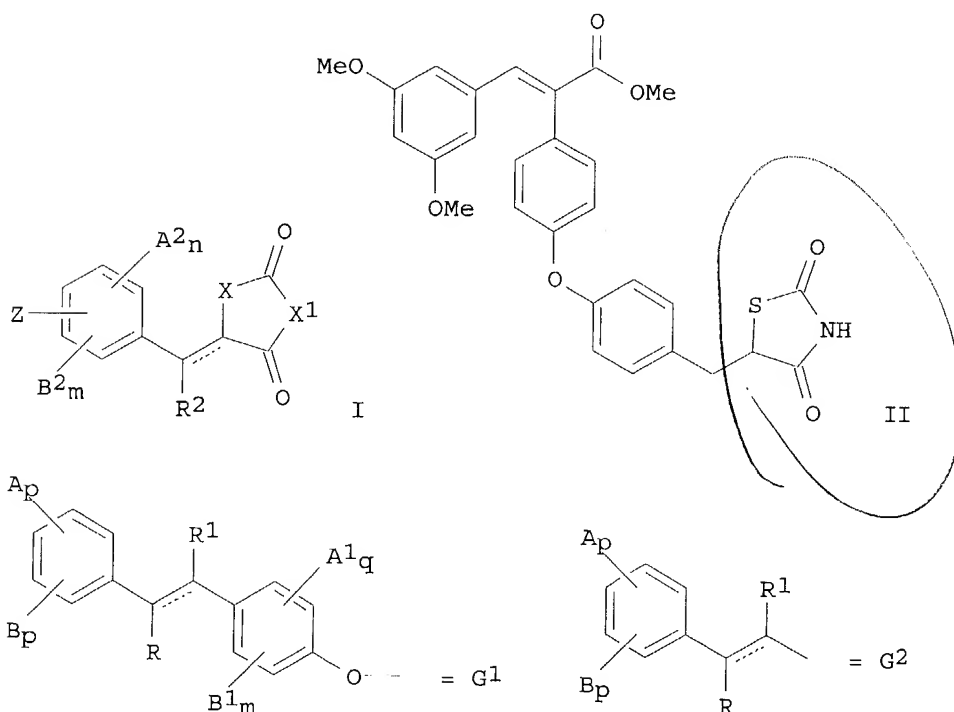
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002025975	A1	20020228	US 2001-785554	20010220 <--
US 6245814	B1	20010612	US 1998-74925	19980508 <--
US 2002032225	A1	20020314	US 2001-843167	20010427 <--
WO 2001095859	A2	20011220	WO 2001-US17950	20010605 <--
WO 2001095859	A3	20030828		

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,

DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
 AU 2001066670 A5 20011224 AU 2001-66670 20010605 <--  
 EP 1360178 A2 20031112 EP 2001-944241 20010605 <--  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, FI, CY, TR  
 US 2003181494 A1 20030925 US 2002-265902 20021008 <--  
 PRIORITY APPLN. INFO.: US 1998-74925 A2 19980508 <--  
 US 1999-287237 A2 19990406 <--  
 US 2000-591105 A2 20000609 <--  
 US 2001-785554 A2 20010220 <--  
 US 2001-843167 A2 20010427 <--  
 WO 2001-US17950 W 20010605 <--  
 OTHER SOURCE(S): MARPAT 136:216745  
 GI

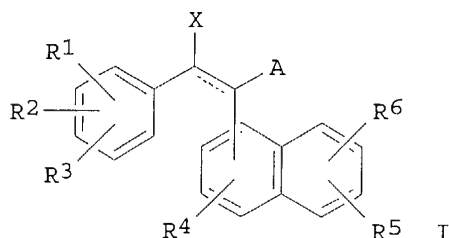


AB Title compds. I [wherein Z = G1, H, A2, B2, or G2; n, m, and q = independently 0-4; p = independently 0-5; R, R1, and R2 = independently H, (un)substituted alkyl or alkenyl, CO2Z1, CO2R3, NH2, NHR3, NR32, OH, OR3, or halo; Z1 = H, Na, K, or other pharmaceutically acceptable counterion; R3 = alkyl or alkenyl; A, A1, and A2 = independently H, acylamino, acyloxy, alkanoyl, alkoxycarbonyl, alkoxy, alkylamino, alkylcarboxylamino, carboxyl, CN, H, or OH; B, B1, and B2 = independently H, acylamino, acyloxy, alkanoyl, alkenoyl, alkoxycarbonyl, alkoxy, alkylamino, alkylcarboxylamino, aroyl, aralkanoyl, carboxyl, CN, halo, or OH; or A and B or A1 and B1 or A2 and B2 together form a methylenedioxy or ethylenedioxy group; X and X1 = independently NH, NR3, O, or S] are provided which are effective in lowering blood glucose level, serum

insulin, **triglyceride**, and free fatty acid levels in animal models of Type II **diabetes**. In contrast to previously reported thiazolidinedione compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity. Thus, II was prepared in five steps by condensation of 3,5-dimethoxybenzaldehyde with 4-hydroxyphenylacetic acid (47%), followed by esterification (97%), etherification with 4-fluorobenzaldehyde (77%), condensation with 2,4-thiazolidinedione (86%), and hydrogenation of the ylidene double bond (40%). Oral administration of II to obese mice caused a 62% drop in blood glucose level. I are useful for the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer, and multiple sclerosis.

L23 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2002:11108 HCAPLUS  
 DOCUMENT NUMBER: 136:69654  
 TITLE: Preparation of diphenylethylene compounds as  
**antidiabetic** agents  
 INVENTOR(S): **Nag, Bishwagit; Dey, Debendranath;**  
**Medicherla, Satyanarayana; Neogi,**  
**Partha**  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 38 pp., Cont.-in-part of U.S.  
 Ser. No. 642,618.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 9  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002002200	A1	20020103	US 2001-777551	20010205 <--
US 6624197	B1	20030923	US 2000-642618	20000817 <--
PRIORITY APPLN. INFO.:			US 2000-180340P	P 20000204 <--
			US 2000-642618	A2 20000817 <--
			US 1998-74925	A2 19980508 <--
OTHER SOURCE(S):		MARPAT 136:69654		
GI				



AB Title compds. I [wherein A = CO<sub>2</sub>R, CONR'R", CN, or COR<sub>7</sub>; X = H, OH, or (un)substituted alkyl or alkenyl; R = H, (ar)alkyl, or aryl; R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>, R<sub>4</sub>, R<sub>5</sub>, R<sub>6</sub>, and R<sub>7</sub> = independently H, (un)substituted alkyl or alkenyl; CO<sub>2</sub>R, NR'R", or CONCR'R"; R' and R" = independently H, alkyl, aryl, OH, alkoxy, acylamino, acyloxy, alkanoyl, alkoxylcarbonyl, halo, NO<sub>2</sub>, SO<sub>2</sub>R'''; CZ<sub>3</sub>; Z = independently H, halo, (halo)alkyl, or SR'''; R''' = H or alkyl; or R<sub>2</sub> and R<sub>3</sub> together or R<sub>5</sub> and R<sub>6</sub> together may be joined to form

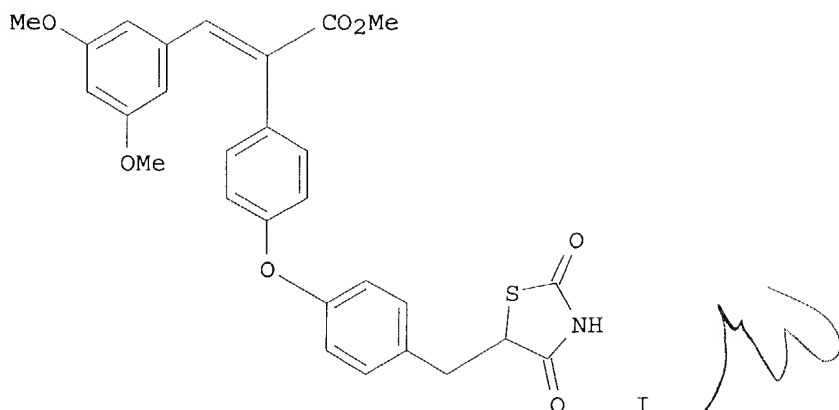
(m)ethylenedioxy; with provisos; and E and Z isomers thereof] were prepared and shown to decrease circulating concns. of glucose when administered orally. For instance, 3,5-dimethoxybenzaldehyde was coupled with p-hydroxyphenyl acetic acid using TEA in acetic anhydride to give (E)-3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid (II), which exhibited glucose-lowering effects for more than 15 days at a dose of 20 mg/kg p.o. Examples also include twenty-six bioassays, such as studies on the effects of II on insulin resistant rats, lipid and leptin concns., PPAR binding, overexpression of the human insulin-like growth factor 1 receptor and human insulin receptor, toxicity, and kinetics of drug absorption. I are orally effective **antidiabetic** agents that normalize glucose and lipid metabolism

L23 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:923567 HCAPLUS  
 DOCUMENT NUMBER: 136:37596  
 TITLE: Preparation and activity of diphenylethylene thiazolidinedione or oxazolidinedione compounds as **antidiabetics** or antiinflammatories  
 INVENTOR(S): **Neogi, Partha; Nag, Bishwajit; Medicherla, Satyanarayana;** Dey, Debendranath  
 PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA  
 SOURCE: PCT Int. Appl., 76 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 9  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001095859	A2	20011220	WO 2001-US17950	20010605 <--
WO 2001095859	A3	20030828		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002025975	A1	20020228	US 2001-785554	20010220 <--
US 2002032225	A1	20020314	US 2001-843167	20010427 <--
AU 2001066670	A5	20011224	AU 2001-66670	20010605 <--
EP 1360178	A2	20031112	EP 2001-944241	20010605 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
PRIORITY APPLN. INFO.:			US 2000-591105	A2 20000609 <--
			US 2001-785554	A2 20010220 <--
			US 2001-843167	A2 20010427 <--
			US 1998-74925	A2 19980508 <--
			US 1999-287237	A2 19990406 <--
			WO 2001-US17950	W 20010605 <--
OTHER SOURCE(S):			MARPAT 136:37596	
GI				





AB Novel diphenylethylene compds. and derivs. thereof containing thiazolidinedione or oxazolidinedione moieties are provided which are effective in lowering blood glucose level, serum insulin, **triglyceride** and free fatty acid levels in animal models of Type II **diabetes**. In contrast to previously reported thiazolidinedione compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity. Thus, (I) was prepared in five steps by condensation of 3,5-dimethoxybenzaldehyde with 4-hydroxyphenylacetic acid followed by esterification and etherification with 4-fluorobenzaldehyde and condensation with 2,4-thiazolidinedione and hydrogenation of the ylidene double bond. Oral administration of I to obese mice caused a 62% drop in blood glucose level. The compds. are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis.

L23 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2001:581654 HCAPLUS  
 DOCUMENT NUMBER: 135:147444  
 TITLE: Novel diphenylethylene compounds  
 INVENTOR(S): **Nag, Bishwajit**; Dey, Debendranath;  
**Medicherla, Satyanarayana**  
 PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA  
 SOURCE: PCT Int. Appl., 55 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 9  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001056382	A1	20010809	WO 2001-US3797	20010205 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,				

DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
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 US 6624197 B1 20030923 US 2000-642618 20000817 <--  
 EP 1251738 A1 20021030 EP 2001-905454 20010205 <--  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
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 JP 2003521500 T2 20030715 JP 2001-556090 20010205 <--  
 PRIORITY APPLN. INFO.: US 2000-180340P P 20000204 <--  
 US 2000-642618 A 20000817 <--  
 US 1998-74925 A2 19980508 <--  
 WO 2001-US3797 W 20010205 <--

OTHER SOURCE(S): MARPAT 135:147444

AB Novel diphenylethylene compds. that are administered orally to decrease circulating concns. of glucose are provided. The effect on insulin resistant rats is also shown. The effects on lipid and leptin concns. are also shown. The compds. are orally effective anti-diabetic agents that may normalize glucose and lipid metabolism in subjects with diabetes.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:359750 HCAPLUS

DOCUMENT NUMBER: 134:348284

TITLE: Phenyl compounds to treat diabetes and associated conditions

INVENTOR(S): Neogi, Partha; Nag, Bishwajit;  
 Lakner, Frederick J.; Dey, Debendranath;  
 Medicherla, Satyanarayana

PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA

SOURCE: PCT Int. Appl., 47 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

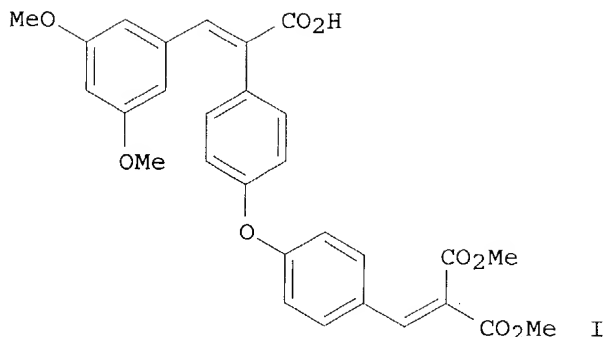
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001034094	A2	20010517	WO 2000-US30927	20001108 <--
WO 2001034094	C2	20020725		
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RW:				
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US 6525093	B1	20030225	US 1999-436047	19991108 <--
AU 2001017607	A5	20010606	AU 2001-17607	20001108 <--
EP 1235785	A2	20020904	EP 2000-980331	20001108 <--
R:				
AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004503464	T2	20040205	JP 2001-536099	20001108 <--
US 2002107285	A1	20020808	US 2002-75442	20020215 <--
PRIORITY APPLN. INFO.:			US 1999-436047	A 19991108 <--
			WO 2000-US30927	W 20001108 <--
OTHER SOURCE(S):				
MARPAT 134:348284				

GI



AB Ph compds. (Markush included) are provided that lower blood glucose concns., lower serum **triglyceride** concns., lower systolic blood pressure, and increase glucose uptake by adipose tissue, but do not affect the expression of PPAR- $\gamma$  by adipose tissue. Compds. of the invention include e.g. I.

L23 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:824099 HCAPLUS

DOCUMENT NUMBER: 133:362623

TITLE: Diphenylethylenes and styrenes for decreasing blood glucose levels

INVENTOR(S): Nag, Bishwajit; Medicherla, Satyanarayana; Dey, Debendranath

PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA

SOURCE: PCT Int. Appl., 27 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

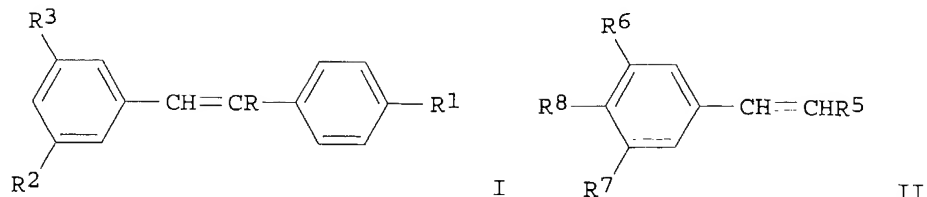
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000069430	A1	20001123	WO 1999-US11001	19990518 <--
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AU 9940857	A1	20001205	AU 1999-40857	19990518 <--
EP 1178788	A1	20020213	EP 1999-924332	19990518 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002544227	T2	20021224	JP 2000-617889	19990518 <--
PRIORITY APPLN. INFO.: WO 1999-US11001 A 19990518 <--				
OTHER SOURCE(S): MARPAT 133:362623				

GI



AB Diphenylethylenes I (R = H, CO<sub>2</sub>H, CO<sub>2</sub>Na, etc.; R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> = H, OH, alkoxy; when R = H and R<sub>2</sub> = R<sub>3</sub> = MeO, R<sub>1</sub> is not OH) and styrenes II (R<sub>5</sub> = H, Me; R<sub>6</sub>, R<sub>7</sub> = H, MeO; R<sub>8</sub> = H, OH) were prepared as **antidiabetic** agents. Thus, reaction of 3,5-dimethoxybenzaldehyde with (4-hydroxyphenyl)acetic acid in AcOH-Et<sub>3</sub>N at 130-140° for 24 h gave I (R = CO<sub>2</sub>H, R<sub>1</sub> = OH, R<sub>2</sub> = R<sub>3</sub> = MeO), which was decarboxylated by refluxing with Cu in quinoline and was converted to the Na salt by reaction with NaOH at room temperature. The styrenes were prepared by Wittig reactions of benzaldehydes. I (R = CO<sub>2</sub>Na, R<sub>1</sub> = OH, R<sub>2</sub> = R<sub>3</sub> = MeO) reduced blood glucose, plasma **triglyceride**, and plasma insulin levels in rats and improved glucose tolerance in insulin-resistant obese rats.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:736478 HCAPLUS

DOCUMENT NUMBER: 131:332116

TITLE: Heterocyclic analogs of diphenylethylene compounds for the treatment of **diabetes**

INVENTOR(S): Neogi, Partha; Nag, Bishwajit; Medicherla, Satyanarayana; Dey, Debendranath

PATENT ASSIGNEE(S): Calyx Therapeutics, Inc., USA

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 9

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9958127	A1	19991118	WO 1999-US9982	19990507 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6245814	B1	20010612	US 1998-74925	19980508 <--
AU 9939741	A1	19991129	AU 1999-39741	19990507 <--
AU 751235	B2	20020808		
EP 1007039	A1	20000614	EP 1999-922836	19990507 <--
EP 1007039	B1	20040303		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				

JP 2002514598 T2 20020521 JP 2000-547978 19990507 <--  
 AT 260906 E 20040315 AT 1999-922836 19990507 <--  
 PRIORITY APPLN. INFO.: US 1998-74925 A 19980508 <--  
 US 1999-287237 A 19990406 <--  
 WO 1999-US9982 W 19990507 <--

OTHER SOURCE(S): MARPAT 131:332116

AB Diphenylethylene compds. containing thiazolidinedione or oxazolidinedione moieties are provided which are effective in lowering blood glucose level, serum insulin, **triglyceride** and free fatty acid levels in animal models of Type II **diabetes**. In contrast to previously reported thiazolidine compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 12 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 2003:162019 BIOSIS

DOCUMENT NUMBER: PREV200300162019

TITLE: Compounds to treat diabetes and associated conditions.

AUTHOR(S): **Neogi, Partha** [Inventor, Reprint Author];  
**Nag, Bishwajit** [Inventor]; **Lakner, Frederick J.** [Inventor]; Dey, Debendranath [Inventor];  
**Medicherla, Satyanarayana** [Inventor]

CORPORATE SOURCE: Hayward, CA, USA

ASSIGNEE: Calyx Therapeutics Inc.

PATENT INFORMATION: US 6525093 February 25, 2003

SOURCE: Official Gazette of the United States Patent and Trademark Office Patents, (Feb 25 2003) Vol. 1267, No. 4.  
<http://www.uspto.gov/web/menu/patdata.html>. e-file.  
 ISSN: 0098-1133 (ISSN print).

DOCUMENT TYPE: Patent

LANGUAGE: English

ENTRY DATE: Entered STN: 26 Mar 2003

Last Updated on STN: 26 Mar 2003

AB Compounds are provided that lower blood glucose concentrations, lower serum **triglyceride** concentrations, lower systolic blood pressure, and increase glucose uptake by adipose tissue, but do not affect the expression of PPAR-gamma by adipose tissue.

L23 ANSWER 13 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 2003:459396 BIOSIS

DOCUMENT NUMBER: PREV200300459396

TITLE: BLX-1002: A new class of orally-active anti-diabetic small molecule with no PPAR-gamma affinity.

AUTHOR(S): Pandey, Bindu [Reprint Author]; Nag, Abhijeet [Reprint Author]; Singh, Ashmika [Reprint Author]; Vargas, Hyang [Reprint Author]; Gutala, Sreekanth [Reprint Author]; Dey, Deben [Reprint Author]; **Nag, Bishwajit** [Reprint Author]

CORPORATE SOURCE: Union City, CA, USA

SOURCE: Diabetes, (2003) Vol. 52, No. Supplement 1, pp. A143. print.

Meeting Info.: **63rd Scientific Sessions of the American Diabetes Association**. New Orleans, LA, USA. June 13-17, 2003. American Diabetes Association.  
 ISSN: 0012-1797 (ISSN print).

DOCUMENT TYPE: **Conference; (Meeting)**

**Conference; (Meeting Poster)**

**Conference; Abstract; (Meeting Abstract)**

LANGUAGE: English

ENTRY DATE: Entered STN: 8 Oct 2003  
Last Updated on STN: 8 Oct 2003

L23 ANSWER 14 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
ACCESSION NUMBER: 2003:531294 BIOSIS  
DOCUMENT NUMBER: PREV200300531302  
TITLE: A nonadipogenic compound BLX-1002 induces glucose uptake in 3T3-L1 cells and has strong anti-hyperglycemic effect in db/db and ob/ob mice.  
AUTHOR(S): Dey, D. [Reprint Author]; Gupta, A.; Pandey, B.; Nag, A. [Reprint Author]; Agarwal, S. K.; **Nag, B.** [Reprint Author]  
CORPORATE SOURCE: Research and Development, Bexel Pharmaceuticals Inc., Union City, CA, USA  
SOURCE: Diabetologia, (August 2003) Vol. 46, No. Supplement 2, pp. A 300. print.  
Meeting Info.: **18th Congress of the International Diabetes Federation.** Paris, France. August 24-29, 2003. International Diabetes Federation.  
CODEN: DBTGAI. ISSN: 0012-186X.  
DOCUMENT TYPE: **Conference; (Meeting)**  
**Conference; Abstract; (Meeting Abstract)**  
LANGUAGE: English  
ENTRY DATE: Entered STN: 12 Nov 2003  
Last Updated on STN: 12 Nov 2003

L23 ANSWER 15 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
ACCESSION NUMBER: 2002:370349 BIOSIS  
DOCUMENT NUMBER: PREV200200370349  
TITLE: SleemaX: A new herbamin formulation as an anti-obese alternative medicine with hypolipidemic and insulin sensitizing properties.  
AUTHOR(S): Nag, Abhijeet [Reprint author]; Nag, Nitish [Reprint author]; **Nag, Bishwajit** [Reprint author]  
CORPORATE SOURCE: BEXEL Biotechnology, Inc., 29552 Union City Blvd., Union City, CA, 94587, USA  
SOURCE: FASEB Journal, (March 22, 2002) Vol. 16, No. 5, pp. A1017. print.  
Meeting Info.: **Annual Meeting of Professional Research Scientists on Experimental Biology.** New Orleans, Louisiana, USA. April 20-24, 2002.  
CODEN: FAJOEC. ISSN: 0892-6638.  
DOCUMENT TYPE: **Conference; (Meeting)**  
**Conference; Abstract; (Meeting Abstract)**  
LANGUAGE: English  
ENTRY DATE: Entered STN: 3 Jul 2002  
Last Updated on STN: 3 Jul 2002

AB Obesity is a chronic disorder characterized by several parameters such as overabundance of adipose tissue, high **triglycerides**, and link with insulin resistance. Obesity is linked with hypertension, coronary heart disease and diabetes. Limited medications are available to tackle this huge growing concern in developed countries. Studies show that a number of herbs and minerals may play a key role in lowering body fat mass in obese people. SleemaX was formulated with two natural product extracts in combination with mineral ions and unusual amino acids. When given orally to ob/ob mice for a period of three weeks, SleemaX lowered body weight by 10% without any change in daily food and water intake. SleemaX reduced hyperinsulinemia by 52%, total cholesterol by 28%, serum **triglycerides** by 42% and basal blood glucose concentration by 44% in ob/ob mice. In a fasting stage, ob/ob mice treated with SleemaX for 2

weeks showed a significant improvement in oral glucose tolerance at all time points. These results indicate that daily oral administration of SleemaX can lower body weight and ameliorate the insulin resistance in mature onset of obesity. The mechanism of SleemaX action is currently being investigated. With no change in food uptake in these animals, SleemaX has the potential as a non-appetite suppressive alternative medicine for the management of obesity.

L23 ANSWER 16 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
 ACCESSION NUMBER: 2002:396559 BIOSIS  
 DOCUMENT NUMBER: PREV200200396559  
 TITLE: Dichol improves glucose homeostasis, insulin sensitivity, and restores lipid balance in two genetic rodent models of type II diabetes.  
 AUTHOR(S): **Nag, Bishwajit** [Reprint author]; **Medicherla, Satya** [Reprint author]; Nag, Abhijeet [Reprint author]  
 CORPORATE SOURCE: BEXEL Biotechnology, Inc., 29552 Union City Blvd., Union City, CA, 94587, USA  
 SOURCE: FASEB Journal, (March 20, 2002) Vol. 16, No. 4, pp. A647-A648. print.  
 Meeting Info.: **Annual Meeting of the Professional Research Scientists on Experimental Biology.** New Orleans, Louisiana, USA. April 20-24, 2002.  
 CODEN: FAJOEC. ISSN: 0892-6638.  
 DOCUMENT TYPE: **Conference; (Meeting)**  
**Conference; Abstract; (Meeting Abstract)**  
 LANGUAGE: English  
 ENTRY DATE: Entered STN: 24 Jul 2002  
 Last Updated on STN: 24 Jul 2002

AB Type II diabetes is a complex metabolic disorder involving hyperglycemia with progressive development of insulin resistance, and is linked with a cascade of other metabolic defects leading to hypertension and hyperlipidemia. Dichol is a herbamin formulation containing two natural product extracts in combination with trace metal ions and relevant amino acids. The efficacy of Dichol was examined in diabetic db/db and ob/ob mice. Single dose oral administration of Dichol for 2 weeks at a dose of 500 mg/kg resulted in >40% and >30% **transient** correction of hyperglycemia in db/db and ob/ob mice. Unlike many antidiabetic drugs where body weight gain occurs, formulated Dichol treatment was attributed with reduction in body weight gain in both ob/ob and db/db mice models. Oral administration of Dichol in db/db and ob/ob mice resulted in improvement in glucose tolerance, lowering of **triglycerides** (50-61%) and total cholesterol (20-52%). In addition, Dichol treatment increased HDL concentrations in db/db mice (32%) but not in ob/ob mice. Long term treatment (15-21 days) with therapeutic dose reduced food intake in both db/db and ob/ob mice. Although the mechanism of Dichol action is not yet defined, results demonstrate the feasibility of discovering a novel insulin sensitizing herbamin that may lead to new alternative therapies for diabetes associated with hyperlipidemia.

L23 ANSWER 17 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
 ACCESSION NUMBER: 2002:134506 BIOSIS  
 DOCUMENT NUMBER: PREV200200134506  
 TITLE: Heterocyclic analogs of diphenylethylene compounds.  
 AUTHOR(S): **Neogi, Partha** [Inventor, Reprint author];  
**Nag, Bishwajit** [Inventor]; **Medicherla, Satyanarayana** [Inventor]; Dey, Debendranath [Inventor]  
 CORPORATE SOURCE: Fremont, CA, USA  
 ASSIGNEE: Calyx Therapeutics Inc., Hayward, CA, USA  
 PATENT INFORMATION: US 6331633 December 18, 2001

SOURCE: Official Gazette of the United States Patent and Trademark  
Office Patents, (Dec. 18, 2001) Vol. 1253, No. 3.  
<http://www.uspto.gov/web/menu/patdata.html>. e-file.  
CODEN: OGUPE7. ISSN: 0098-1133.

DOCUMENT TYPE: Patent  
LANGUAGE: English  
ENTRY DATE: Entered STN: 6 Feb 2002  
Last Updated on STN: 26 Feb 2002

AB Novel diphenylethylene compounds containing thiazolidinedione or oxazolidinedione moieties are provided which are effective in lowering blood glucose level, serum insulin, **triglyceride** and free fatty acid levels in animal models of Type II diabetes. In contrast to previously reported thiazolidine compounds, known to lower leptin levels, the present compound increase leptin levels and have no known liver toxicity.

L23 ANSWER 18 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 2001:297270 BIOSIS

DOCUMENT NUMBER: PREV200100297270

TITLE: Evidence for the interaction of a small molecule with insulin receptor using surface plasmon resonance.

AUTHOR(S): Dey, Deben [Reprint author]; **Neogi, Partha** [Reprint author]; **Nag, Bishwajit** [Reprint author]

CORPORATE SOURCE: Calyx Therapeutics Inc., 3525 Breakwater Avenue, Hayward, CA, 94545, USA

SOURCE: FASEB Journal, (March 7, 2001) Vol. 15, No. 4, pp. A526.  
print.  
Meeting Info.: **Annual Meeting of the Federation of American Societies for Experimental Biology on Experimental Biology 2001**. Orlando, Florida, USA. March 31-April 04, 2001.  
CODEN: FAJOEC. ISSN: 0892-6638.

DOCUMENT TYPE: **Conference; (Meeting)**  
**Conference; Abstract; (Meeting Abstract)**

LANGUAGE: English

ENTRY DATE: Entered STN: 20 Jun 2001  
Last Updated on STN: 19 Feb 2002

AB CLX-0901, a synthetic water-soluble analog of a compound (CLX-0900) isolated from the heartwood of a plant, has been shown to lower blood glucose, **triglyceride** and free fatty acid concentrations in several animal models of type II diabetes. In addition, we have previously shown that CLX-0901, like insulin, stimulated rapid glucose uptake (within 30 minutes) in primary rat adipocytes and this uptake is inhibited by known PI 3-kinase inhibitors. CLX-0901, in a manner similar to insulin, also stimulated Akt activation and GLUT-4 **translocation** in 3T3-L1 adipocytes. To demonstrate whether these findings are due to direct interaction of CLX-0901 with the insulin receptor (IR), a cell-free system that utilizes surface plasmon resonance measurements was employed. The IR and the insulin-like growth factor binding protein-1 (IGFBP-1), used as a control surface, were immobilized by amine coupling to the dextran matrix of a CM5 sensor chip, and the remaining active groups were blocked with 1 M ethanolamine (pH 8.5). Varying concentrations of either insulin or CLX-0901 in PBS were injected at a flow rate of 20 micro liter/min for 2 minutes over the immobilized surfaces. Dose response curves of insulin and CLX-0901 were very similar, but the affinity of CLX-0901 for IR was 1000-fold less than that of insulin. Addition of CLX-0901 to the IGFBP-1 surface did not induce a response. To further **confirm** the specificity of these interactions, insulin-like growth factor-1 (IGF-1) was also injected over both surfaces. Passage of IGF-1 over an IGFBP-1 surface induced a



response to IGFBP-1 but not to IR. Several additional compounds known not to interact with IR, such as tolbutamide and an eighteen-amino-acid peptide with insulin-like activity (CLX-0100), showed no interaction with any of the surfaces. These results provide evidence that CLX-0901 selectively binds to the insulin receptor.

L23 ANSWER 19 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
ACCESSION NUMBER: 2001:449945 BIOSIS  
DOCUMENT NUMBER: PREV200100449945  
TITLE: Antidiabetic properties of CLX-090700, a  
non-thiazolidinedione compound.  
AUTHOR(S): Gowri, Maya [Reprint author]; Dey, Deben [Reprint author];  
Cheng, Jin [Reprint author]; Sen, Ananda [Reprint author];  
**Medicherla, Satya** [Reprint author]; **Neogi,**  
**Partha** [Reprint author]  
CORPORATE SOURCE: Hayward, CA, USA  
SOURCE: Diabetes, (June, 2001) Vol. 50, No. Supplement 2, pp. A69.  
print.  
Meeting Info.: **61st Scientific Sessions of the**  
**American Diabetes Association.** Philadelphia,  
Pennsylvania, USA. June 22-26, 2001. American Diabetes  
Association.  
CODEN: DIAEAZ. ISSN: 0012-1797. ✓  
DOCUMENT TYPE: **Conference; (Meeting)**  
**Conference; Abstract; (Meeting Abstract)**  
LANGUAGE: English  
ENTRY DATE: Entered STN: 19 Sep 2001  
Last Updated on STN: 22 Feb 2002

L23 ANSWER 20 OF 20 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN  
ACCESSION NUMBER: 1995:194325 BIOSIS  
DOCUMENT NUMBER: PREV199598208625  
TITLE: Co-regulation of very low density lipoprotein metabolism by  
dietary carbohydrate and cholesterol in hamsters.  
AUTHOR(S): Almario, R. [Reprint author]; **Medicherla, S.;**  
Kasim-Karakas, S. E.  
CORPORATE SOURCE: Univ. California, Davis, CA, USA  
SOURCE: FASEB Journal, (1995) Vol. 9, No. 3, pp. A440.  
Meeting Info.: Experimental Biology 95, Part I. Atlanta,  
Georgia, USA. April 9-13, 1995.  
CODEN: FAJOEC. ISSN: 0892-6638.  
DOCUMENT TYPE: **Conference; (Meeting)**  
**Conference; Abstract; (Meeting Abstract)**  
LANGUAGE: English  
ENTRY DATE: Entered STN: 5 May 1995  
Last Updated on STN: 15 May 1995

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2/4

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STRUCTURE FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1  
DICTIONARY FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1

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Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

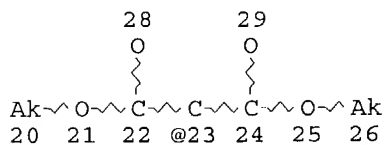
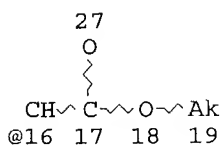
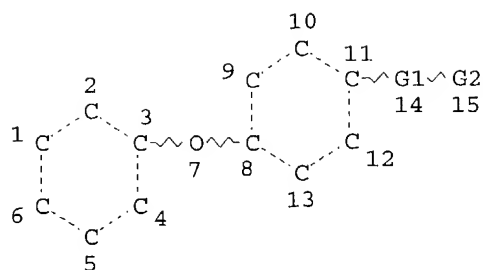
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LAST RELOADED: Jul 16, 2004 (20040716/UP).

=> d que l18

L11 STR



VAR G1=CH2/16

VAR G2=CH2/16/23

NODE ATTRIBUTES:

NSPEC IS RC AT 7

CONNECT IS E1 RC AT 27

CONNECT IS E1 RC AT 28

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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

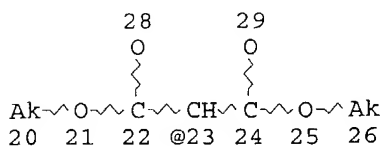
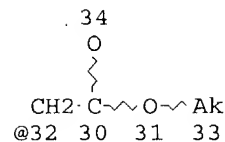
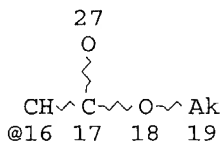
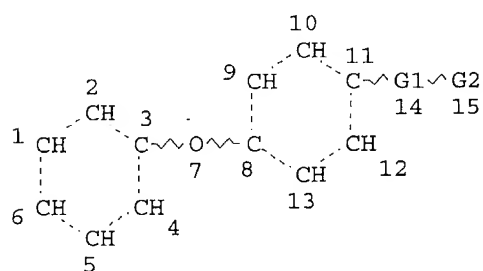
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NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

L13 4813 SEA FILE=REGISTRY SSS FUL L11

L16 STR



VAR G1=CH2/16

VAR G2=CH3/32/23

NODE ATTRIBUTES:

NSPEC IS RC AT 7

CONNECT IS E1 RC AT 27

CONNECT IS E1 RC AT 28

CONNECT IS E1 RC AT 29  
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DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE  
L18 10 SEA FILE=REGISTRY SUB=L13 SSS FUL L16

=> fil reg

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STRUCTURE FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1  
DICTIONARY FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1

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Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> analyze l18  
ENTER ANSWER NUMBER OR RANGE (1-):1-  
ENTER DISPLAY CODE (CHEM) OR ?:lc  
L20 ANALYZE L18 1- LC : 6 TERMS

=> d  
L20 ANALYZE L18 1- LC : 6 TERMS

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2	10	10	100.00	CAPLUS
3	4	4	40.00	BEILSTEIN
4	3	3	30.00	TOXCENTER
5	3	3	30.00	USPATFULL
6	2	2	20.00	CASREACT

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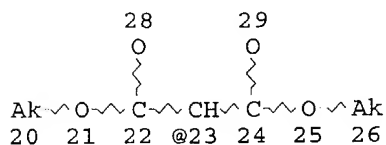
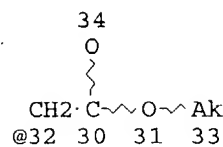
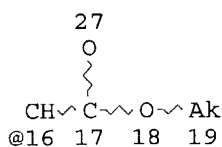
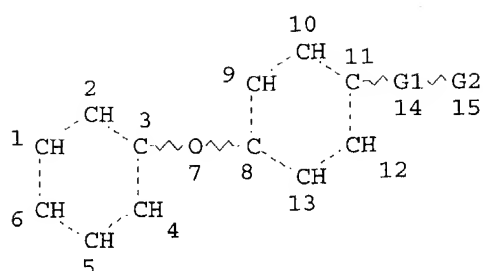
FILE COVERS 1771 TO 2003.  
\*\*\* FILE CONTAINS 8,997,153 SUBSTANCES \*\*\*

>>> PLEASE NOTE: Reaction data and substance data are stored in  
separate documents and can not be searched together in one  
query.  
Reaction data for BEILSTEIN compounds may be displayed  
immediately with the display codes PRE (preparations) and REA  
(reactions). A substance answer set retrieved after the search  
for a chemical name, a molecular formula or a structure search  
for example can be restricted to compounds with available  
reaction information by concatenation with PRE/FA, REA/FA or  
more general with RX/FA. The BEILSTEIN Registry Number (BRN)  
is the link between a BEILSTEIN compound and belonging reactions.  
For more detailed reaction searches BRNs can be selected from  
substance answer sets and searched in the next step as reaction  
partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN).  
After a search for reaction details substance documents  
associated with reactants or products may be retrieved by  
searching RX.PBRNs or RX.RBRNs as BRNs. <<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\*\*\*\*\*  
\* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. \*  
\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE \*  
\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*  
\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

=> d que 122  
L16 STR



VAR G1=CH2/16

VAR G2=CH3/32/23

NODE ATTRIBUTES:

NSPEC IS RC AT 7

CONNECT IS E1 RC AT 27

CONNECT IS E1 RC AT 28

CONNECT IS E1 RC AT 29

CONNECT IS E1 RC AT 34

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

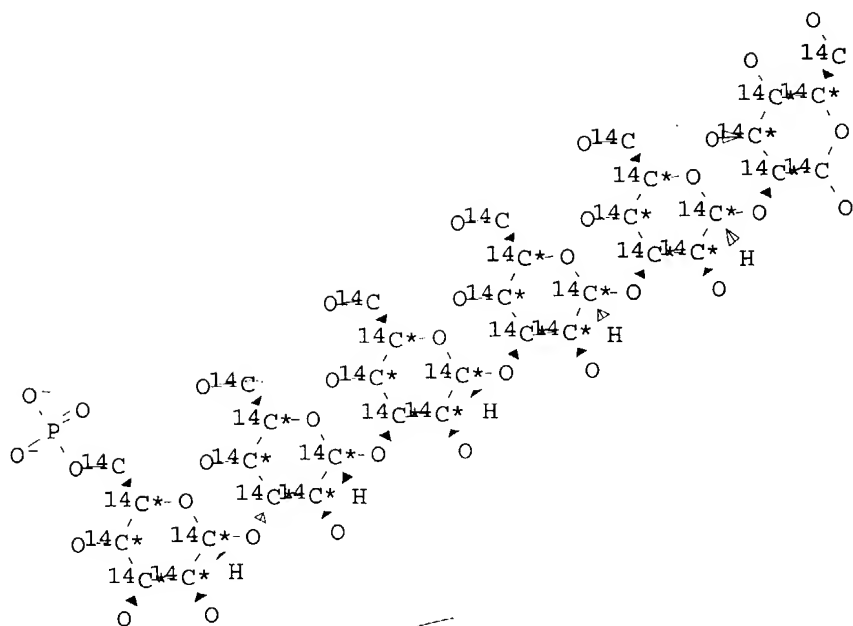
L21 8 SEA FILE=BEILSTEIN SSS FUL L16

L22 4 SEA FILE=BEILSTEIN ABB=ON PLU=ON L21 NOT RN/FA

=> d ide 122

L22 ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	9317926
Lin. Struct. Formula (LSF):	(14)C36H61O34P(2-)
Molec. Formula (MF):	C36 H61 O34 P
Molecular Weight (MW):	1068.83
Lawson Number (LN):	17647, 1122
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7867777
Tautomer ID (TAUTID):	8747803
Entry Date (DED):	2003/04/17
Update Date (DUPD):	2003/04/17



## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d l22 rx

L22 ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 9208376  
 Reactant BRN (.RBRN): 6409585  
 Reactant (.RCT): U-14C-Glucose  
 Product BRN (.PBRN): 9315848, 9316930, 9317534, 9317926

Product (.PRO): (14)C18H31O19P(2-), (14)C24H41O24P(2-),  
(14)C30H51O29P(2-), (14)C36H61O34P(2-)  
No. of React. Details (.NVAR): 1

## Reaction Details:

RX

Reaction RID (.RID): 9208376.1  
Reaction Classification (.CL): Multistage  
Nr. of Stages (.SNR): 2  
Stage 1  
Reagent (.RGT): Pichia hostii NRRL Y-2448 culture, KH2PO4  
Solvent (.SOL): H2O  
Time (.TIM): 15.5 hour(s)  
Temperature (.T): 28 Cel  
Stage 2  
Reagent (.RGT): HCl  
Solvent (.SOL): H2O  
Time (.TIM): 6 hour(s)  
pH Value (.PH): 2  
Other Conditions (.COND): Heating  
Note(s) (.COM): Further byproducts given. Title compound  
not separated from byproducts

## Reference(s):

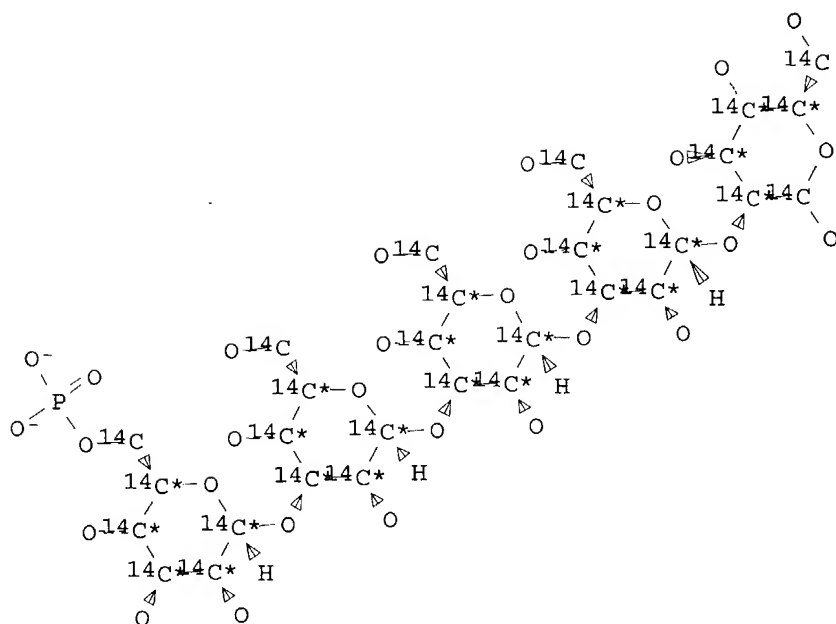
1. Ferro, Vito; Li, Caiping; Wang, Bin; Fewings, Kym; King, Andrew R.;  
Hammond, Edward; Creese, Brian R., J. Labelled Compd. Radiopharm., CODEN:  
JLCRD4, 45(9), <2002>, 747 - 754; BABS-6369742

=> d l22 ide 2

L22 ANSWER 2 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9317534  
Lin. Struct. Formula (LSF): (14)C30H51O29P(2-)  
Molec. Formula (MF): C30 H51 O29 P  
Molecular Weight (MW): 906.69  
Lawson Number (LN): 17647, 1122  
File Segment (FS): Stereo compound  
Compound Type (CTYPE): heterocyclic  
Constitution ID (CONSID): 7867414  
Tautomer ID (TAUTID): 8747344  
Entry Date (DED): 2003/04/17  
Update Date (DUPD): 2003/04/17





## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

d 122 rx 2

L22 ANSWER 2 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 9208376  
 Reactant BRN (.RBRN): 6409585  
 Reactant (.RCT): U-14C-Glucose

*Handwritten signature: NPA*

Product BRN (.PBRN): 9315848, 9316930, 9317534, 9317926  
Product (.PRO): (14)C18H31O19P(2-), (14)C24H41O24P(2-),  
(14)C30H51O29P(2-), (14)C36H61O34P(2-)  
No. of React. Details (.NVAR): 1

## Reaction Details:

RX

Reaction RID (.RID): 9208376.1  
Reaction Classification (.CL): Multistage  
Nr. of Stages (.SNR): 2  
Stage 1  
Reagent (.RGT): Pichia hostii NRRL Y-2448 culture, KH2PO4  
Solvent (.SOL): H2O  
Time (.TIM): 15.5 hour(s)  
Temperature (.T): 28 Cel  
Stage 2  
Reagent (.RGT): HCl  
Solvent (.SOL): H2O  
Time (.TIM): 6 hour(s)  
pH Value (.PH): 2  
Other Conditions (.COND): Heating  
Note(s) (.COM): Further byproducts given. Title compound  
not separated from byproducts

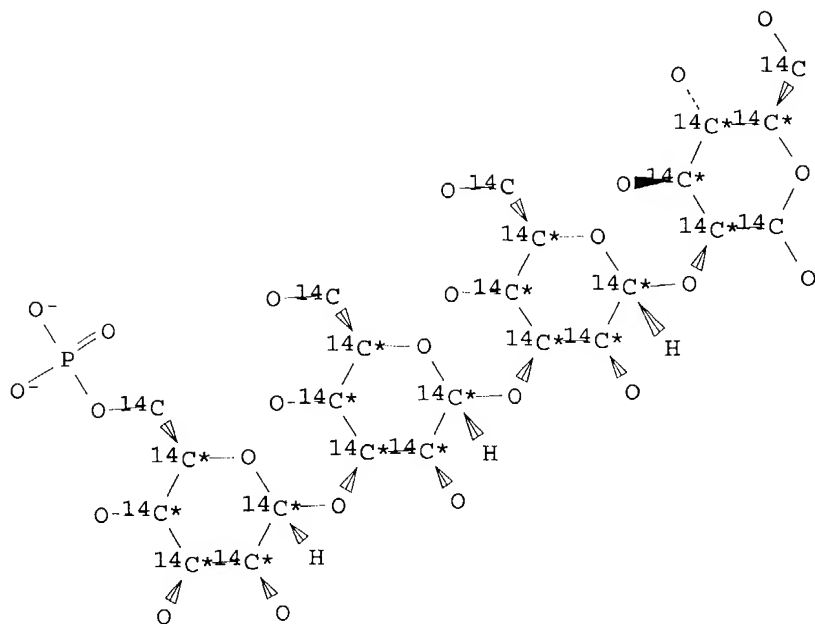
## Reference(s):

1. Ferro, Vito; Li, Caiping; Wang, Bin; Fewings, Kym; King, Andrew R.;  
Hammond, Edward; Creese, Brian R., J.Labelled Compd.Radiopharm., CODEN:  
JLCRD4, 45(9), <2002>, 747 - 754; BABS-6369742

=&gt; d 122 ide 3

L22 ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9316930  
Lin. Struct. Formula (LSF): (14)C24H41O24P(2-)  
Molec. Formula (MF): C24 H41 O24 P  
Molecular Weight (MW): 744.55  
Lawson Number (LN): 17647, 1122  
File Segment (FS): Stereo compound  
Compound Type (CTYPE): heterocyclic  
Constitution ID (CONSID): 7866922  
Tautomer ID (TAUTID): 8746329  
Entry Date (DED): 2003/04/17  
Update Date (DUPD): 2003/04/17



## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=>

=> d l22 rx 3

L22 ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:

RX

Reaction ID (.ID): 9208376  
 Reactant BRN (.RBRN): 6409585

Reactant (.RCT): U-14C-Glucose  
Product BRN (.PBRN): 9315848, 9316930, 9317534, 9317926  
Product (.PRO): (14)C18H31O19P(2-), (14)C24H41O24P(2-),  
(14)C30H51O29P(2-), (14)C36H61O34P(2-)  
No. of React. Details (.NVAR): 1

## Reaction Details:

RX

Reaction RID (.RID): 9208376.1  
Reaction Classification (.CL): Multistage  
Nr. of Stages (.SNR): 2  
Stage 1  
Reagent (.RGT): Pichia hostii NRRL Y-2448 culture, KH2PO4  
Solvent (.SOL): H2O  
Time (.TIM): 15.5 hour(s)  
Temperature (.T): 28 Cel  
Stage 2  
Reagent (.RGT): HCl  
Solvent (.SOL): H2O  
Time (.TIM): 6 hour(s)  
pH Value (.PH): 2  
Other Conditions (.COND): Heating  
Note(s) (.COM): Further byproducts given. Title compound  
not separated from byproducts

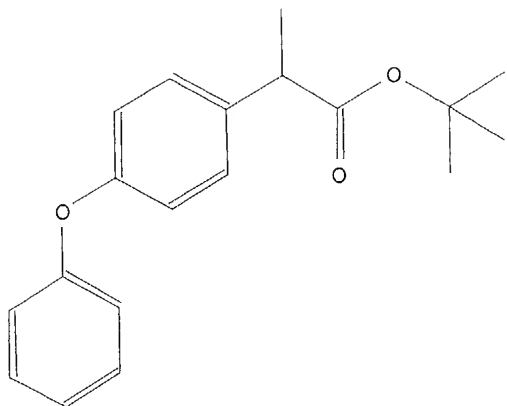
## Reference(s):

1. Ferro, Vito; Li, Caiping; Wang, Bin; Fewings, Kym; King, Andrew R.;  
Hammond, Edward; Creese, Brian R., J.Labelled Compd.Radiopharm., CODEN:  
JLCRD4, 45(9), <2002> 747 - 754; BABS-6369742

=&gt; d ide l22 4

L22 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 8984649  
Chemical Name (CN): tert-butyl  $\alpha$ -(4-diphenoxy)propionate  
Autonom Name (AUN): 2-(4-phenoxy-phenyl)-propionic acid  
tert-butyl ester  
Molec. Formula (MF): C19 H22 O3  
Molecular Weight (MW): 298.38  
Lawson Number (LN): 11705, 5219, 318  
Compound Type (CTYPE): isocyclic  
Constitution ID (CONSID): 7596317  
Tautomer ID (TAUTID): 8448692  
Entry Date (DED): 2002/04/29  
Update Date (DUPD): 2002/04/29



## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
NMR	Nuclear Magnetic Resonance	3

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXPRO	Substance is Reaction Product	2

=> d rx l22 4

L22 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

## Reaction:

RX

Reaction ID (.ID): 8938769  
 Reactant BRN (.RBRN): 1747857, 1948803  
 Reactant (.RCT): propionic acid tert-butyl ester,  
 (4-chloro-phenyl)-phenyl ether  
 Product BRN (.PBRN): 8984649  
 Product (.PRO): 2-(4-phenoxy-phenyl)-propionic acid  
 tert-butyl ester  
 No. of React. Details (.NVAR): 1

## Reaction Details:

RX

Reaction RID (.RID): 8938769.1  
Reaction Classification (.CL): Preparation  
Yield (.YDT): 54 percent (BRN=8984649)  
Reagent (.RGT): Pd2(dba)3, LiHMDS, 2-P(t-Bu)2-2'-NMe2-1,1'-biphenyl  
Solvent (.SOL): toluene  
Time (.TIM): 3 hour(s)  
Temperature (.T): 80 Cel  
Reference(s):  
1. Moradi, Wahed A.; Buchwald, Stephen L., J.Amer.Chem.Soc., CODEN: JACSAT, 123(33), <2001>, 7996 - 8002; BABS-6324113

## Reaction:

RX

Reaction ID (.ID): 8934433  
Reactant BRN (.RBRN): 1747857, 1308972  
Reactant (.RCT): propionic acid tert-butyl ester,  
1-bromo-4-phenoxy-benzene  
Product BRN (.PBRN): 8984649  
Product (.PRO): 2-(4-phenoxy-phenyl)-propionic acid  
tert-butyl ester  
No. of React. Details (.NVAR): 1

## Reaction Details:

RX

Reaction RID (.RID): 8934433.1  
Reaction Classification (.CL): Preparation  
Yield (.YDT): 71 percent (BRN=8984649)  
Reagent (.RGT): Pd(OAc)2, LiHMDS, 2-PCy2-2'-NMe2-1,1'-biphenyl  
Solvent (.SOL): toluene  
Time (.TIM): 2 hour(s)  
Temperature (.T): 80 Cel  
Reference(s):  
1. Moradi, Wahed A.; Buchwald, Stephen L., J.Amer.Chem.Soc., CODEN: JACSAT, 123(33), <2001>, 7996 - 8002; BABS-6324113

=&gt; FIL STNGUIDE

FILE 'STNGUIDE' ENTERED AT 15:18:25 ON 20 JUL 2004  
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Jul 16, 2004 (20040716/UP).

=&gt;

=> fil lreg

FILE 'LREGISTRY' ENTERED AT 15:11:10 ON 20 JUL 2004  
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LREGISTRY IS A STATIC LEARNING FILE

=> fil reg

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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1  
DICTIONARY FILE UPDATES: 19 JUL 2004 HIGHEST RN 713066-32-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

=> fil beilst

FILE 'BEILSTEIN' ENTERED AT 15:11:25 ON 20 JUL 2004  
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FILE RELOADED ON OCTOBER 20, 2002  
FILE LAST UPDATED ON JUNE 15, 2004

FILE COVERS 1771 TO 2003.

\*\*\* FILE CONTAINS 8,997,153 SUBSTANCES \*\*\*

>>> PLEASE NOTE: Reaction data and substance data are stored in  
separate documents and can not be searched together in one  
query.

Reaction data for BEILSTEIN compounds may be displayed  
immediately with the display codes PRE (preparations) and REA  
(reactions). A substance answer set retrieved after the search  
for a chemical name, a molecular formula or a structure search  
for example can be restricted to compounds with available  
reaction information by concatenation with PRE/FA, REA/FA or  
more general with RX/FA. The BEILSTEIN Registry Number (BRN)  
is the link between a BEILSTEIN compound and belonging reactions.  
For more detailed reaction searches BRNs can be selected from

substance answer sets and searched in the next step as reaction partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN). After a search for reaction details substance documents associated with reactants or products may be retrieved by searching RX.PBRNs or RX.RBRNs as BRNs. <<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\*\*\*\*\*  
\* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. \*  
\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE \*  
\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*  
\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 15:11:34 ON 20 JUL 2004  
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FILE COVERS 1907 - 20 Jul 2004 VOL 141 ISS 4  
FILE LAST UPDATED: 19 Jul 2004 (20040719/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> fil uspatfull

FILE 'USPATFULL' ENTERED AT 15:11:42 ON 20 JUL 2004  
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 20 Jul 2004 (20040720/PD)  
FILE LAST UPDATED: 20 Jul 2004 (20040720/ED)  
HIGHEST GRANTED PATENT NUMBER: US6766528  
HIGHEST APPLICATION PUBLICATION NUMBER: US2004139525  
CA INDEXING IS CURRENT THROUGH 20 Jul 2004 (20040720/UPCA)  
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 20 Jul 2004 (20040720/PD)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2004  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2004

>>> USPAT2 is now available. USPATFULL contains full text of the <<<  
>>> original, i.e., the earliest published granted patents or <<<  
>>> applications. USPAT2 contains full text of the latest US <<<  
>>> publications, starting in 2001, for the inventions covered in <<<



```
>>> USPATFULL. A USPATFULL record contains not only the original <<<
>>> published document but also a list of any subsequent <<<
>>> publications. The publication number, patent kind code, and <<<
>>> publication date for all the US publications for an invention <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<
>>> records and may be searched in standard search fields, e.g., /PN, <<<
>>> /PK, etc. <<<
```

```
>>> USPATFULL and USPAT2 can be accessed and searched together <<<
>>> through the new cluster USPATALL. Type FILE USPATALL to <<<
>>> enter this cluster. <<<
>>> <<<
>>> Use USPATALL when searching terms such as patent assignees, <<<
>>> classifications, or claims, that may potentially change from <<<
>>> the earliest to the latest publication. <<<
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This file contains CAS Registry Numbers for easy and accurate substance identification.

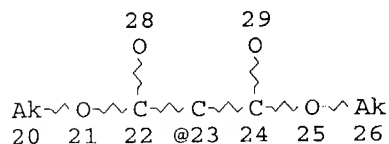
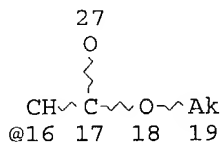
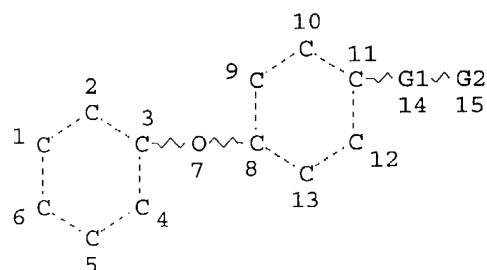
=> FIL STNGUIDE

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FILE CONTAINS CURRENT INFORMATION.  
 LAST RELOADED: Jul 16, 2004 (20040716/UP).

=> d que 119  
 L11

STR



```
VAR G1=CH2/16
VAR G2=CH2/16/23
NODE ATTRIBUTES:
NSPEC   IS RC      AT    7
CONNECT IS E1     RC AT  27
CONNECT IS E1     RC AT  28
CONNECT IS E1     RC AT  29
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
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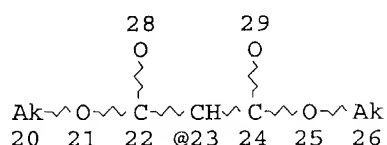
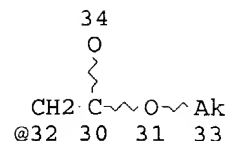
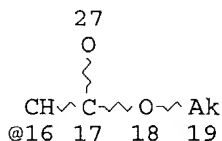
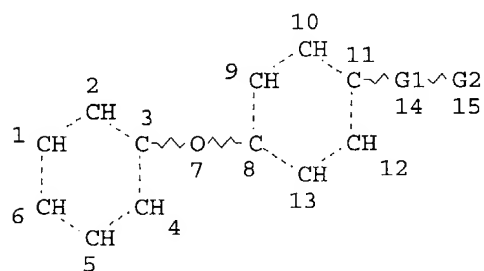
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

L13 4813 SEA FILE=REGISTRY SSS FUL L11

L16 STR



VAR G1=CH2/16

VAR G2=CH3/32/23

NODE ATTRIBUTES:

NSPEC IS RC AT 7

CONNECT IS E1 RC AT 27

CONNECT IS E1 RC AT 28

CONNECT IS E1 RC AT 29

CONNECT IS E1 RC AT 34

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 34

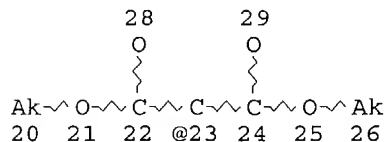
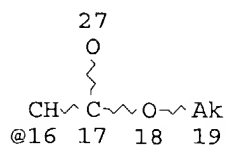
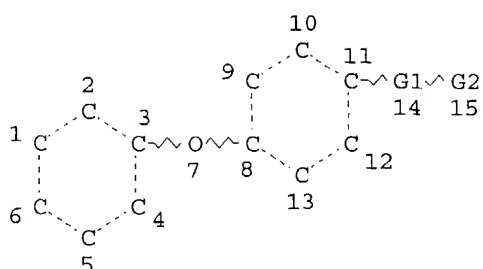
STEREO ATTRIBUTES: NONE

L18 10 SEA FILE=REGISTRY SUB=L13 SSS FUL L16

L19 13 SEA FILE=HCAPLUS ABB=ON PLU=ON L18

=> d que l23

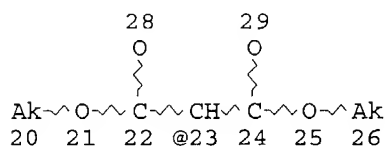
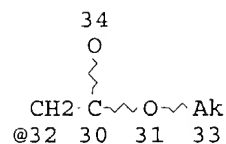
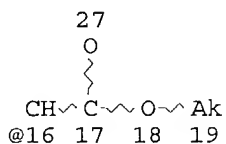
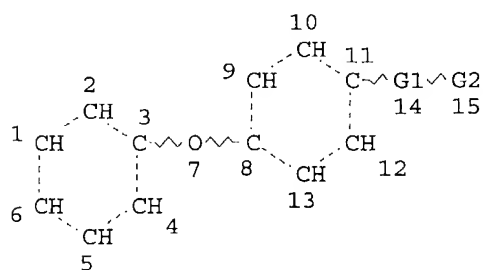
L11 STR



VAR G1=CH2/16  
 VAR G2=CH2/16/23  
 NODE ATTRIBUTES:  
 NSPEC IS RC AT 7  
 CONNECT IS E1 RC AT 27  
 CONNECT IS E1 RC AT 28  
 CONNECT IS E1 RC AT 29  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE  
 L13 4813 SEA FILE=REGISTRY SSS FUL L11  
 L16 STR



VAR G1=CH2/16  
 VAR G2=CH3/32/23  
 NODE ATTRIBUTES:  
 NSPEC IS RC AT 7  
 CONNECT IS E1 RC AT 27  
 CONNECT IS E1 RC AT 28

CONNECT IS E1 RC AT 29  
CONNECT IS E1 RC AT 34  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE  
L18 10 SEA FILE=REGISTRY SUB=L13 SSS FUL L16  
L23 2 SEA FILE=USPATFULL ABB=ON PLU=ON L18

=> dup rem l19 l23

FILE 'HCAPLUS' ENTERED AT 15:12:17 ON 20 JUL 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE 'USPATFULL' ENTERED AT 15:12:17 ON 20 JUL 2004  
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)  
PROCESSING COMPLETED FOR L19  
PROCESSING COMPLETED FOR L23  
L24 15 DUP REM L19 L23 (0 DUPLICATES REMOVED)  
ANSWERS '1-13' FROM FILE HCAPLUS  
ANSWERS '14-15' FROM FILE USPATFULL

=> d iall hitstr 1-13

L24 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2001:546122 HCAPLUS  
DOCUMENT NUMBER: 135:257023  
ENTRY DATE: Entered STN: 29 Jul 2001  
TITLE: Palladium-catalyzed  $\alpha$ -arylation of esters  
AUTHOR(S): Moradi, Wahed A.; Buchwald, Stephen L.  
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of  
Technology, Cambridge, MA, 02139, USA  
SOURCE: Journal of the American Chemical Society (2001),  
123(33), 7996-8002  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
CLASSIFICATION: 25-18 (Benzene, Its Derivatives, and Condensed  
Benzenoid Compounds)  
OTHER SOURCE(S): CASREACT 135:257023  
ABSTRACT:

A new and simple one-pot procedure for the palladium-catalyzed intermol.  $\alpha$ -arylation of esters is described. A number of esters, e.g. MeCO<sub>2</sub>CMe<sub>3</sub>, can be functionalized with a wide range of aryl bromides, e.g. 2-MeC<sub>6</sub>H<sub>4</sub>Br, using Pd(OAc)<sub>2</sub> or Pd<sub>2</sub>(dba)<sub>3</sub> and bulky electron-rich o-biphenyl phosphines. Under the reaction conditions, using LiHMDS as base,  $\alpha$ -arylation proceeds at room temperature or at 80°C with very good yields and high selectivities for monoarylation. Important nonsteroidal antiinflammatory drug derivs. such as (±)-naproxen tert-Bu ester and (±)-flurbiprofen tert-Bu ester can be prepared in 79% and 86% yield, resp. The catalyst system based on the o-biphenyl containing a dimethylamino group and di-tert-butylphosphine moiety is also active for the  $\alpha$ -arylation of esters using aryl chlorides. Furthermore, using a

bipnaphthyl di-tert-butylphosphine ligand, the  $\alpha$ -arylation of trisubstituted ester enolates can be accomplished to provide compds. that have quaternary centers.

SUPPL. TERM: arylation ester palladium biphenyl binaphthyl ligand catalyst

INDEX TERM: Arylation  
Arylation catalysts  
(palladium-catalyzed  $\alpha$ -arylation of esters with aryl halides using biphenyl/binaphthyl phosphine ligands)

INDEX TERM: Aryl halides  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(palladium-catalyzed  $\alpha$ -arylation of esters with aryl halides using biphenyl/binaphthyl phosphine ligands)

INDEX TERM: 3375-31-3, palladium(II) acetate 51364-51-3, Pd2(dba)3  
213697-53-1 224311-49-3 224311-52-8  
ROLE: CAT (Catalyst use); USES (Uses)  
(palladium-catalyzed  $\alpha$ -arylation of esters with aryl halides using biphenyl/binaphthyl phosphine ligands)

INDEX TERM: 92-66-0, 1-Bromo-4-phenylbenzene 95-46-5, 2-Bromotoluene  
101-55-3, 1-Bromo-4-phenoxybenzene 101-97-3, Ethyl 2-phenylacetate 103-64-0, 1-Bromo-2-phenylethene  
106-38-7, 4-Bromotoluene 106-43-4, 4-Chlorotoluene  
108-37-2, 1-Bromo-3-chlorobenzene 401-78-5, 1-Bromo-3-(trifluoromethyl)benzene 460-00-4, 1-Bromo-4-fluorobenzene 540-88-5, tert-Butyl acetate  
576-22-7, 1-Bromo-2,6-dimethylbenzene 580-13-2, 2-Bromonaphthalene 586-77-6, 1-Bromo-4-(dimethylamino)benzene 623-12-1, 1-Chloro-4-methoxybenzene  
2039-88-5, 1-Bromo-2-vinylbenzene 2308-38-5, tert-Butyl butanoate 5111-65-9, 2-Bromo-6-methoxynaphthalene  
5892-99-9 7005-72-3, 1-Chloro-4-phenoxybenzene  
7073-94-1, 1-Bromo-2-(isopropyl)benzene 7452-79-1, Ethyl 2-methylbutanoate 20487-40-5, tert-Butyl propanoate  
23786-14-3 41604-19-7, 1,1'-Biphenyl, 4-bromo-2-fluoro  
59247-47-1, tert-Butyl 4-bromobenzoate  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(palladium-catalyzed  $\alpha$ -arylation of esters with aryl halides using biphenyl/binaphthyl phosphine ligands)

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138623-00-4P 138623-03-7P 362523-40-8P 362523-41-9P  
362523-42-0P 362523-43-1P 362523-44-2P 362523-45-3P  
362523-46-4P 362523-47-5P **362523-48-6P**  
362523-49-7P 362523-50-0P 362523-51-1P 362523-52-2P  
362523-53-3P 362523-54-4P 362523-55-5P 362523-56-6P  
362523-57-7P 362523-58-8P  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(palladium-catalyzed  $\alpha$ -arylation of esters with aryl halides using biphenyl/binaphthyl phosphine ligands)

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S): (1) Agnelli, F; Tetrahedon Lett 1998, V39, P8807 HCAPLUS  
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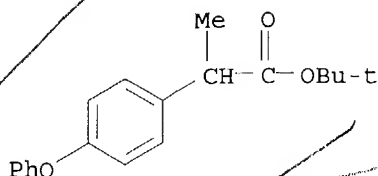
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IT 362523-48-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(palladium-catalyzed  $\alpha$ -arylation of esters with aryl halides  
using biphenyl/binaphthyl phosphine ligands)

RN 362523-48-6 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -methyl-4-phenoxy-, 1,1-dimethylethyl ester  
(9CI) (CA INDEX NAME)



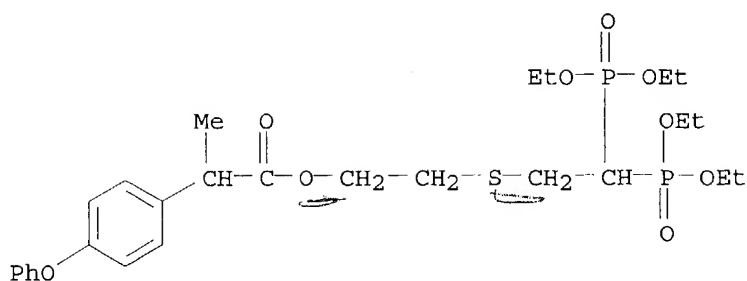
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L24 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2000:136796 HCAPLUS  
 DOCUMENT NUMBER: 132:265251  
 ENTRY DATE: Entered STN: 29 Feb 2000  
 TITLE: Synthesis of antiinflammatory analgesics  
 bisphosphonate compounds  
 AUTHOR(S): Zheng, Hu; Wu, Yong; Weng, Ling-Ling  
 CORPORATE SOURCE: School of Pharmacy, West China University of Medical  
 Sciences, Chengdu, 610041, Peop. Rep. China  
 SOURCE: Hecheng Huaxue (1999) 7(4), 427-429  
 CODEN: HEHUE2; ISSN: 1005-1511  
 PUBLISHER: Hecheng Huaxue Bianjibu  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 CLASSIFICATION: 29-7 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 1

ABSTRACT: Bisphosphonates, e.g. HOCH<sub>2</sub>CH<sub>2</sub>SCH<sub>2</sub>CH[P(O)(OEt)<sub>2</sub>]<sub>2</sub>, have bone-seeking affinity, antiarthritic and analgesic activity as well. In order to research bone-targeted leading compds. with high activity of antihypertrophic arthritics and low toxicity, five antiinflammatory analgesics-bisphosphonate compds. were designed and synthesized. MSM

SUPPL. TERM: antiinflammatory analgesic bis phosphonate prepn;  
 bisphosphonate prepn antiinflammatory analgesic  
 INDEX TERM: Antiarthritics  
 (antihypertrophic; synthesis of antiinflammatory  
 analgesics bisphosphonate compds.)  
 INDEX TERM: Anti-inflammatory agents  
 (nonsteroidal; synthesis of antiinflammatory analgesics  
 bisphosphonate compds.)  
 INDEX TERM: 6145-33-1P 121001-81-8P 177172-94-0P 182919-44-4P  
 263565-12-4P 263565-13-5P 263565-14-6P  
**263565-15-7P** 263565-16-8P 263565-17-9P  
 ROLE: BAC (Biological activity or effector, except adverse);  
 BSU (Biological study, unclassified); SPN (Synthetic  
 preparation); BIOL (Biological study); PREP (Preparation)  
 (synthesis of antiinflammatory analgesics bisphosphonate  
 compds.)

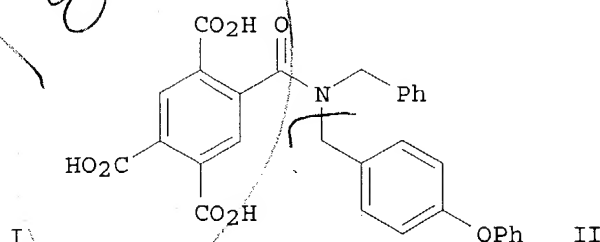
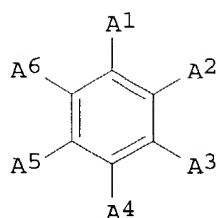
IT **263565-15-7P**  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); SPN (Synthetic preparation); BIOL (Biological  
 study); PREP (Preparation)  
 (synthesis of antiinflammatory analgesics bisphosphonate compds.)  
 RN 263565-15-7 HCAPLUS  
 CN Benzeneacetic acid,  $\alpha$ -methyl-4-phenoxy-, 2-[[2,2-  
 bis(diethoxyphosphinyl)ethyl]thio]ethyl ester (9CI) (CA INDEX NAME) M



L24 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1997:44662 HCAPLUS  
 DOCUMENT NUMBER: 126:59751  
 ENTRY DATE: Entered STN: 22 Jan 1997  
 TITLE: Preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors  
 INVENTOR(S): Baker, William R.; Rosenberg, Saul H.; Fung, K. L. Anthony; Rockway, Todd W.; Fakhoury, Stephen A.; Garvey, David S.; Donner, B. Gregory; O'Connor, Stephen J.; Prasad, Rajnandan N.; Shen, Wang; Stout, David M.; Sullivan, Gerard M.  
 PATENT ASSIGNEE(S): Abbott Laboratories, USA  
 SOURCE: PCT Int. Appl., 241 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 INT. PATENT CLASSIF.:  
 MAIN: C07C233-73  
 SECONDARY: C07C233-65; C07C235-38; C07D257-04; C07C275-42; C07C335-22; C07C233-12; C07D333-20  
 CLASSIFICATION: 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 1  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9634851	A1	19961107	WO 1996-US6193	19960502
W: AU, CA, JP, KR, MX				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5783593	A	19980721	US 1996-633262	19960429
AU 9656731	A1	19961121	AU 1996-56731	19960502
PRIORITY APPLN. INFO.:			US 1995-429095	19950503
			US 1996-633262	19960429
			US 1993-147708	19931104
			US 1994-289711	19940909
			US 1994-322783	19941018
			WO 1996-US6193	19960502
OTHER SOURCE(S):			MARPAT 126:59751	
GRAPHIC IMAGE:				





## ABSTRACT:

Title compds. [e.g., I; A1 = ZCONR1R2, A2, A4, and A5 or A2 and A4 or A3 and A4 = (protected) CO<sub>2</sub>H and the other A<sub>n</sub> = H; R1 = (chloro)benzyl, (CH<sub>2</sub>)<sub>2</sub>-4Ph, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>(OPh)-4; R2 = (CH<sub>2</sub>)<sub>1</sub>-2C<sub>6</sub>H<sub>4</sub>(OPh)-4; Z = bond, NR, O; R = H, (cyclo)alkyl, aralkyl, cycloalkylalkyl] were prepared. Thus, 4-(PhO)C<sub>6</sub>H<sub>4</sub>CHO was reductively aminated by H<sub>2</sub>CH<sub>2</sub>Ph and the product amidated by 1,2,4,5-benzenetetracarboxylic dianhydride to give title compound II. Data for in vitro inhibition of protein farnesyltransferase by selected I were given.

SUPPL. TERM: carboxybenzamide squalene synthetase protein  
farnesyltransferase inhibitor

INDEX TERM: Artery, disease  
(coronary, restenosis, prevention; preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

INDEX TERM: Ras proteins  
ROLE: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(farnesylation; preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

INDEX TERM: Antitumor agents  
(preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

INDEX TERM:	185047-82-9P	185047-83-0P	185047-84-1P	185047-85-2P
	185047-86-3P	185047-87-4P	185047-88-5P	185047-89-6P
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185050-25-3P	185051-65-4P		

ROLE: BAC (Biological activity or effector, except adverse);  
 BSU (Biological study, unclassified); SPN (Synthetic  
 preparation); THU (Therapeutic use); BIOL (Biological  
 study); PREP (Preparation); USES (Uses)

(preparation of di- and tricarboxybenzamides and analogs as  
 squalene synthetase and protein farnesyltransferase  
 inhibitors)

INDEX TERM: 131384-38-8, Protein farnesyltransferase

ROLE: BPR (Biological process); BSU (Biological study,  
 unclassified); BIOL (Biological study); PROC (Process)

(preparation of di- and tricarboxybenzamides and analogs as  
 squalene synthetase and protein farnesyltransferase  
 inhibitors)

INDEX TERM: 170433-63-3P, 1,2-Benzenedicarboxylic acid,  
 4-hydroxymethyl-, dimethyl ester

ROLE: BYP (Byproduct); PREP (Preparation)

(preparation of di- and tricarboxybenzamides and analogs as  
 squalene synthetase and protein farnesyltransferase  
 inhibitors)

INDEX TERM: 61-54-1, 3-(2-Aminoethyl)indole 65-49-6, 4-Aminosalicylic  
 acid 67-36-7, 4-Phenoxybenzaldehyde 85-44-9,

1,3-Isobenzofurandione 89-32-7 89-51-0, Homophthalic

acid 89-57-6, 5-Aminosalicylic acid 89-93-0,

2-Methylbenzylamine 93-09-4, 2-Naphthoic acid 93-55-0,

Propiophenone 95-48-7, reactions 95-65-8,

3,4-Dimethylphenol 96-32-2, Methyl bromoacetate 99-63-8,

1,3-Benzenedicarbonyl dichloride 100-20-9,

1,4-Benzenedicarbonyl dichloride 100-39-0, Benzyl bromide

100-46-9, Benzylamine, reactions 100-51-6, Benzyl alcohol,

reactions 100-52-7, Benzaldehyde, reactions 100-81-2,  
 3-Methylbenzylamine 101-53-1, 4-Hydroxydiphenylmethane  
 103-49-1, Dibenzylamine 103-63-9, Phenethyl bromide  
 106-44-5, 4-Methylphenol, reactions 106-48-9,  
 4-Chlorophenol 108-39-4, 3-Methylphenol, reactions  
 118-31-0, 1-Naphthylmethylamine 138-25-0 150-76-5,  
 4-Methoxyphenol 459-57-4, 4-Fluorobenzaldehyde 527-60-6,  
 2,4,6-Trimethylphenol 552-30-7 556-56-9, Allyl iodide  
 569-51-7, 1,2,3-Benzenetricarboxylic acid 610-22-0,  
 Dimethyl 4-nitrophthalate 699-98-9, 2,3-  
 Pyridinedicarboxylic anhydride 703-59-3, Homophthalic  
 anhydride 1204-28-0, 4-Chlorocarbonylphthalic anhydride  
 1758-46-9, 2-Phenoxyethylamine 1955-46-0,  
 3-Nitroisophthalic acid monomethyl ester 2038-57-5,  
 Benzenepropanamine 2045-79-6, 2-Methoxyphenethylamine  
 2217-40-5, 1-Amino-1,2,3,4-Tetrahydronaphthalene  
 2270-20-4, 5-Phenylpentanoic acid 2393-23-9,  
 4-Methoxybenzylamine 2420-87-3, [5,5'-Biisobenzofuran]-  
 1,1',3,3'-tetrone 2421-28-5 2426-87-1,  
 4-Benzyloxy-3-methoxybenzaldehyde 2672-58-4,  
 1,3,5-Benzenetricarboxylic acid, trimethyl ester  
 2687-43-6, O-Benzylhydroxylamine hydrochloride 2740-83-2,  
 3-Trifluoromethylbenzylamine 2835-06-5 2975-41-9,  
 2-Aminoindane 3048-01-9, 2-Trifluoromethylbenzylamine  
 3082-77-7, L-Methionine ethyl ester 3113-72-2,  
 5-Methyl-2-nitrobenzoic acid 3132-99-8,  
 3-Bromobenzaldehyde 3218-02-8, Cyclohexanemethanamine  
 3218-36-8, 4-Phenylbenzaldehyde 3669-48-5 3711-01-1,  
 2,3,6,7-Naphthalenetetracarboxylic dianhydride 3731-51-9,  
 2-Pyridylmethylamine 3731-52-0, 3-Pyridylmethylamine  
 3731-53-1, 4-Pyridylmethylamine 3939-09-1,  
 2,4-Difluorobenzonitrile 4360-51-4, 1-Amino-3-phenyl-2-  
 propene 4393-09-3, 2,3-Dimethoxybenzylamine 4397-53-9,  
 4-Benzyloxybenzaldehyde 4442-59-5, 1,4-Benzodioxan-2-  
 methylamine 4821-94-7, 4,5-Dimethoxyphthalic anhydride  
 5326-47-6, 2-Amino-5-iodobenzoic acid 5372-81-6, Dimethyl  
 aminoterephthalate 5470-84-8, 4-Benzyloxybutyraldehyde  
 5736-88-9, 4-Butoxybenzaldehyde 5870-38-2, Diethyl  
 2,5-dihydroxyterephthalate 5927-18-4,  
 Trimethylphosphonoacetate 6050-13-1, Diphenic anhydride  
 6287-38-3, 3,4-Dichlorobenzaldehyde 6328-74-1,  
 4-Phenoxyphenylacetic acid 6850-57-3, 2-Methoxybenzylamine  
 6921-34-2, Benzylmagnesium chloride 7355-22-8,  
 5-Bromo-2,4-dihydroxybenzoic acid 7409-30-5,  
 4-Nitrobenzylamine 7617-76-7, 3-Phenoxypropylamine  
 7745-93-9, 2-Bromo-4-nitrotoluene 13214-66-9,  
 4-Phenylbutylamine 17532-66-0, 1,2-Benzenediacetic acid,  
 diethyl ester 18655-51-1, 3-(2-Methoxyphenyl)propylamine  
 19014-14-3 19434-34-5, 2-Phenoxybenzaldehyde 20116-65-8,  
 Dimethyl 4-methylphthalate 20781-22-0 22117-85-7  
 22440-62-6 22479-95-4, Dimethyl 4-hydroxyphthalate  
 24541-01-3, 4-Chromanone oxime 24850-33-7,  
 Allyltributyltin 26759-46-6 27757-85-3,  
 2-Thiophenemethanamine 28994-41-4, 2-  
 Hydroxydiphenylmethane 34698-41-4, 1-Aminoindane  
 37806-29-4, 2-Ethoxybenzylamine 37806-49-8,  
 Benzenemethanamine, 2-(3-methylbutoxy)- 37806-66-9  
 39515-51-0, 3-Phenoxybenzaldehyde 39590-27-7,  
 Benzeneethanamine, 2-ethoxy- 40663-68-1,  
 4-Allyloxybenzaldehyde 42116-44-9, N-tert-

Butoxycarbonylbenzenemethanamine 58332-00-6 60728-41-8  
 69770-20-3, 3-(4-Chlorophenoxy)benzaldehyde 69770-23-6,  
 3-(4-tert-Butylphenoxy)benzaldehyde 72235-53-1,  
 3,4-Difluorobenzylamine 79124-75-7, 3-(4-Methylphenoxy)benzaldehyde 79124-76-8,  
 3-(3,4-Dichlorophenoxy)benzaldehyde 88088-95-3,  
 Tris(1-benzotriazolyl)methane 107624-14-6,  
 Benzenemethanamine, 2-phenoxy- 165534-79-2, Dimethyl  
 iodoterephthalate 169943-62-8 169943-64-0 171350-07-5  
 171350-08-6 184229-19-4, 4-Phenoxy-3-chlorobenzaldehyde  
 185051-61-0 185051-62-1 185051-63-2 185051-64-3,  
 N-Benzyl-2-fluorenylmethylamine

ROLE: RCT (Reactant); RACT (Reactant or reagent)

(preparation of di- and tricarboxybenzamides and analogs as  
 squalene synthetase and protein farnesyltransferase  
 inhibitors)

INDEX TERM:

2215-84-1P 3786-39-8P 3898-66-6P 4315-09-7P,  
 4-Nitrobenzene-1,3-dicarboxylic acid 16426-64-5P  
 19241-40-8P 20116-67-0P, 1,2-Benzenedicarboxylic acid,  
 4-bromomethyl-, dimethyl ester 29710-58-5P 38588-64-6P,  
 1,3,5-Benzenetricarboxylic acid, dimethyl ester  
 39585-32-5P, Benzeneacetic acid, 2-carboxy-5-nitro-  
 40172-06-3P, N-(3,4-Dichlorobenzyl)ethanolamine  
 46253-86-5P 51832-31-6P, Dimethyl 4-aminophthalate  
 52446-51-2P, 2-(4-Phenoxyphenyl)ethanol 53981-38-7P,  
 4-Aminochroman 60313-18-0P 63746-12-3P, Dimethyl  
 4-aminoisophthalate 64481-29-4P 67402-72-6P  
 68872-14-0P 69048-70-0P, Dimethyl 4-nitroisophthalate  
 74733-34-9P 76784-89-9P, Benzeneacetic acid,  
 5-amino-2-(methoxycarbonyl)-, methyl ester 79807-86-6P  
 91345-28-7P 91963-85-8P 100959-22-6P, Methyl  
 2-bromo-4-nitrobenzoate 110786-89-5P, 1,2-  
 Benzenedicarboxylic acid, 4-mercapto-, dimethyl ester  
 129951-06-0P, Benzenebutanamine, N-phenylmethyl-  
 136534-67-3P, Benzenepentanamine, N-phenylmethyl-  
 138408-68-1P, Methyl 4-hydroxy-2-methoxy-5-vinylbenzoate  
 144146-84-9P, N-Benzyl-5-phenylpentanamide 147810-06-8P  
 169943-97-9P, N-Benzyl-N-(4-phenoxybenzyl)amine  
 170433-65-5P, Dimethyl 4-(carboxymethyl)phthalate  
 179056-63-4P 179098-29-4P 184033-42-9P,  
 4-tert-Butoxycarbonylamino-2-hydroxybenzoic acid  
 184228-76-0P 184228-77-1P 184228-78-2P 184228-79-3P  
 185050-26-4P 185050-27-5P 185050-28-6P 185050-29-7P  
 185050-30-0P 185050-31-1P 185050-32-2P,  
 2-Cyano-5-iodobenzoic acid 185050-33-3P 185050-34-4P  
 185050-35-5P 185050-36-6P 185050-37-7P 185050-38-8P  
 185050-39-9P 185050-40-2P 185050-41-3P 185050-42-4P  
 185050-43-5P 185050-44-6P 185050-45-7P 185050-46-8P  
 185050-47-9P 185050-48-0P 185050-49-1P 185050-50-4P  
 185050-51-5P 185050-52-6P 185050-53-7P 185050-54-8P  
 185050-55-9P 185050-56-0P 185050-57-1P 185050-58-2P  
 185050-59-3P 185050-60-6P 185050-61-7P 185050-62-8P  
 185050-63-9P 185050-64-0P 185050-65-1P 185050-66-2P  
 185050-67-3P 185050-68-4P 185050-69-5P 185050-70-8P  
 185050-71-9P 185050-72-0P 185050-73-1P 185050-74-2P  
 185050-75-3P 185050-76-4P 185050-77-5P, Methyl  
 5-bromo-4-hydroxy-2-methoxybenzoate 185050-78-6P  
 185050-79-7P, Methyl 2-methoxy-4,5-divinylbenzoate  
 185050-80-0P, 2-Methoxy-4,5-divinylbenzoic acid  
 185050-81-1P 185050-82-2P 185050-83-3P 185050-84-4P

185050-85-5P 185050-86-6P 185050-87-7P 185050-88-8P  
 185050-89-9P 185050-90-2P 185050-91-3P 185050-92-4P  
 185050-93-5P 185050-94-6P, Methyl 4-tert-  
 Butoxycarbonylamino-2-hydroxyBenzoate 185050-95-7P  
 185050-96-8P 185050-97-9P 185050-98-0P 185050-99-1P  
 185051-00-7P 185051-01-8P **185051-02-9P**  
 185051-03-0P 185051-04-1P 185051-05-2P 185051-06-3P  
 185051-07-4P 185051-08-5P 185051-09-6P 185051-10-9P  
 185051-11-0P 185051-12-1P 185051-13-2P 185051-14-3P  
 185051-15-4P 185051-16-5P 185051-17-6P 185051-18-7P  
 185051-19-8P 185051-20-1P 185051-21-2P 185051-22-3P  
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 185051-47-2P 185051-48-3P 185051-49-4P 185051-50-7P  
 185051-51-8P 185051-52-9P 185051-53-0P 185051-54-1P  
 185051-55-2P 185051-56-3P 185051-57-4P 185051-58-5P  
 185051-59-6P 185051-60-9P 185051-67-6P 185230-57-3P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation of di- and tricarboxybenzamides and analogs as  
 squalene synthetase and protein farnesyltransferase  
 inhibitors)

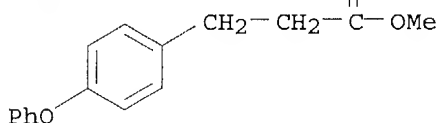
IT **185051-02-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation of di- and tricarboxybenzamides and analogs as squalene  
 synthetase and protein farnesyltransferase inhibitors)

RN 185051-02-9 HCAPLUS

CN Benzenepropanoic acid, 4-phenoxy-, methyl ester (9CI) (CA INDEX NAME)



L24 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:442116 HCAPLUS

DOCUMENT NUMBER: 121:42116

ENTRY DATE: Entered STN: 23 Jul 1994

TITLE: Study on the source of nonvolatile mutagenic organics  
 in the water of East Lake and the tap water from it

AUTHOR(S): Tian, Shizhong; Huang, Zhidan; Deng, Nansheng; Zhang,  
 Jiayao; Zhao, Pihong; Xiao, Mei; Liu, Dazhi; Zhizhong,  
 Jing; Meilan, Wang; Xizhao, Yuan

CORPORATE SOURCE: Dep. Environ. Sci., Wuhan Univ., Wuhan, 430072, Peop.  
 Rep. China

SOURCE: Zhongguo Huanjing Kexue (1993), 13(2), 100-5  
 CODEN: ZHKKEI; ISSN: 1000-6923

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

CLASSIFICATION: 61-2 (Water)

## Section cross-reference(s): 4, 10

## ABSTRACT:

A total of 102 organic pollutants (alkylbenzenes, polycyclic aromatic hydrocarbons, phthalic esters, etc.) in East Lake and the tap water from it were identified by gas chromatog.-mass spectrometry. Ames test results showed that they have mutagenicity to TA98, and are direct mutagens. Model test of chlorination of humic acid or fulvic acid showed that humics of low concentration in water do not form nonvolatile mutagenic orgs. and nonvolatile mutagenic orgs. in the tap water from East Lake.

SUPPL. TERM: org water pollution East Lake China; Salmonella typhimurium toxicity org lake pollution; Ames test toxicity org water pollution

INDEX TERM: Water pollution  
(by organic compds., of lake water and potable water, Salmonella typhimurium toxicity in relation to, of East Lake, China)

INDEX TERM: Organic compounds, biological studies  
ROLE: BIOL (Biological study)  
(lake water and potable water pollution by, Salmonella typhimurium toxicity in relation to, of East Lake, China)

INDEX TERM: Toxicity  
(of organic compds. in polluted lake water and potable water, to Salmonella typhimurium strain TA-98, Ames test determination of, of East Lake, China)

INDEX TERM: Salmonella typhimurium  
(strain TA-98, polluted lake and potable water toxicity to, Ames test for, of East Lake, China)

INDEX TERM: 57-10-3, Hexadecanoic acid, biological studies 64-19-7, Acetic acid, biological studies 67-66-3, Trichloromethane, biological studies 71-43-2, Benzene, biological studies 75-27-4, Bromodichloromethane 75-65-0, Tert-Butanol, biological studies 84-66-2, Diethyl phthalate 84-69-5, Diisobutyl phthalate 84-74-2, Dibutyl phthalate 86-73-7, Fluorene 91-20-3, Naphthalene, biological studies 95-16-9, Benzothiazole 95-50-1, o-Dichlorobenzene 100-41-4, Ethylbenzene, biological studies 100-42-5, biological studies 100-52-7, Benzaldehyde, biological studies 106-46-7, p-Dichlorobenzene 108-88-3, Toluene, biological studies 108-90-7, Chlorobenzene, biological studies 110-54-3, Hexane, biological studies 110-82-7, Cyclohexane, biological studies 110-93-0, 6-Methyl-5-heptene-2-one 111-27-3, Hexanol, biological studies 111-65-9, Octane, biological studies 111-84-2, Nonane 112-30-1, Decanol 112-95-8, Eicosane 117-81-7, Dioctyl phthalate 120-12-7, Anthracene, biological studies 124-48-1, Dibromochloromethane 128-37-0, 2,6-Ditert-butyl-4-methylphenol, biological studies 128-39-2, 2,6-Di-tert-butylphenol 131-11-3 140-29-4, Benzylcyanide 206-44-0, Fluoranthene 486-25-9, 9H-Fluoren-9-one 489-84-9 535-77-3, 1-Methyl-3-isopropylbenzene 541-73-1, m-Dichlorobenzene 544-63-8, Tetradecanoic acid, biological studies 593-45-3, Octadecane 629-78-7, Heptadecane 629-92-5, Nonadecane 629-94-7, Heneicosane 629-97-0, Docosane 646-31-1, Tetracosane 678-26-2, Perfluoropentane 719-22-2 763-93-9, 3-Hexen-2-one 814-78-8 934-34-9, Benzothiazolone 937-30-4 1138-52-9, 3,5-Di-tert-butylphenol 1331-43-7, Diethylcyclohexane 1569-50-2,

3-Pentene-2-ol 1689-78-7, 2-tert-Butylthiophene  
 2142-64-5 2219-82-1, 2-tert-Butyl-6-methylphenol  
 2245-30-9 2444-28-2, 2,6-Di-tert-butyl-1,4-benzenediol  
 4130-42-1, 2,6-Di-tert-butyl-4-ethylphenol 4281-40-7  
 4562-27-0, 4-1H)-Pyrimidinone 4675-87-0 4920-99-4,  
 1-Ethyl-3-isopropylbenzene 7507-89-3 11071-47-9,  
 Isooctene 12002-48-1, Trichlorobenzene 15356-74-8  
 18794-47-3 19377-95-8 24270-68-6, 1,1,2,3-  
 Tetrafluoropropane 25377-83-7, Octene 25378-22-7,  
 Dodecene 25495-91-4, Bromohexane 27138-19-8,  
 Ethylnaphthalene 27195-67-1, Dimethylcyclohexane  
 27400-77-7, Nonadecene 27400-79-9, Heneicosene  
 28351-09-9, Dimethylbenzaldehyde 28804-88-8,  
 Dimethylnaphthalene 29253-36-9, Isopropylnaphthalene  
 29512-02-5, 1-Methoxy-1-butene 29730-67-4, Docosene  
 34314-83-5, 4-Methyl-2,3-dihydrofuran 34464-40-9,  
 Isononane 34970-00-8, Iodobromochloromethane  
**36207-23-5** 53951-50-1, Ethylbenzaldehyde  
 58501-92-1 61923-54-4, 2-Penten-2-ol 62808-70-2  
 103502-85-8 156000-89-4 156057-47-5  
 ROLE: BIOL (Biological study)  
 (lake water and potable water pollution by, Salmonella  
 typhimurium toxicity in relation to, of East Lake, China)

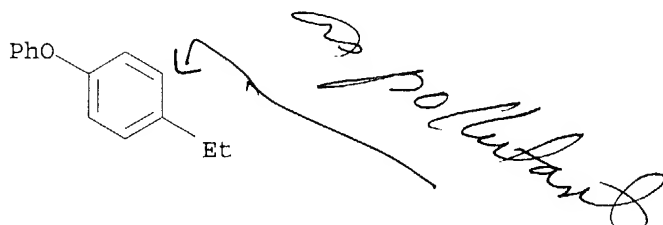
IT 36207-23-5

RL: BIOL (Biological study)

(lake water and potable water pollution by, Salmonella typhimurium  
 toxicity in relation to, of East Lake, China)

RN 36207-23-5 HCAPLUS

CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



L24 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:206735 HCAPLUS

DOCUMENT NUMBER: 112:206735

ENTRY DATE: Entered STN: 26 May 1990

TITLE: Preparation of  $\alpha$ -arylacetic acid derivatives by  
electrochemical oxidation

INVENTOR(S): Shono, Tatsuya; Matsumura, Isahiro

PATENT ASSIGNEE(S): Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

INT. PATENT CLASSIF.:

MAIN: C25B003-02

CLASSIFICATION: 72-9 (Electrochemistry)

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01222078	A2	19890905	JP 1988-50233	19880302

PRIORITY APPLN. INFO.:

JP 1988-50233

19880302

OTHER SOURCE(S):

MARPAT 112:206735

## ABSTRACT:

A method for preparing ACRR1COOR2 (A = aryl, (condensed) heterocyclic group, R, R1 = H, alkyl, alicyclic group, unsatd. hydrocarbon group, aryl, aralkyl; R2 = H or lower alkyl) involves electrochem. oxidation of ACOCHRR1 in the presence of I (or its compound) and an acetalization agent.

SUPPL. TERM: arylacetic acid prepn electrochem oxidn ketone

INDEX TERM: Oxidation, electrochemical

(of ketones, in preparation of arylacetic acid derivs.)

INDEX TERM: 74-88-4, uses and miscellaneous 149-73-5 7553-56-2,

Iodine, uses and miscellaneous

ROLE: PROC (Process)

(electrochem. oxidation of ketones in presence of, for preparation of arylacetic acid derivs.)

INDEX TERM: 75-30-9 75-47-8 591-50-4 3240-34-4 7553-56-2,  
Iodine, uses and miscellaneous 7681-11-0, Potassium iodide  
(KI), uses and miscellaneous 7758-05-6 10034-85-2,  
Hydriodic acid 12027-06-4, Ammonium iodide ((NH4)I)  
16029-98-4

ROLE: PROC (Process)

(electrochem. oxidation of ketones in presence of, in

preparation

of arylacetic acid derivs.)

INDEX TERM: 93-55-0 98-86-2, reactions 495-40-9 582-62-7

611-70-1 712-50-5 889-26-9 1515-95-3 2700-47-2

6315-96-4 10342-83-3 52129-98-3 59771-24-3

66952-37-2 80336-83-0 114012-26-9 120703-45-9

126916-32-3 126934-92-7 126934-93-8

ROLE: RCT (Reactant); RACT (Reactant or reagent)

(electrochem. oxidation of, in preparation of arylacetic acid derivs.)

INDEX TERM: 101-41-7P 2294-71-5P 17380-78-8P 30012-51-2P

31508-44-8P 50415-73-1P 52263-88-4P 57421-64-4P

57625-74-8P 59235-36-8P 61566-34-5P 66202-87-7P

72615-27-1P 73913-50-5P 83636-46-8P 103392-12-7P

120703-46-0P 125670-62-4P 126934-94-9P

**126934-95-0P** 126934-96-1P

ROLE: PREP (Preparation)

(preparation of, electrochem., by oxidation of ketone derivs.)

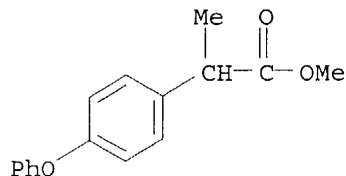
IT **126934-95-0P**

RL: PREP (Preparation)

(preparation of, electrochem., by oxidation of ketone derivs.)

RN 126934-95-0 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -methyl-4-phenoxy-, methyl ester (9CI) (CA  
INDEX NAME)



L24 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:97962 HCAPLUS



DOCUMENT NUMBER: 112:97962  
ENTRY DATE: Entered STN: 18 Mar 1990  
TITLE: Reactivity of ring-substituted ethylbenzenes in reactions with cumylperoxy radicals  
AUTHOR(S): Efimova, I. V.; Matvienko, A. G.; Opeida, I. A.  
CORPORATE SOURCE: Inst. Fiz.-Org. Khim. Uglekhim., Donetsk, USSR  
SOURCE: Zhurnal Organicheskoi Khimii (1989), 25(4), 801-4  
CODEN: ZORKAE; ISSN: 0514-7492  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
CLASSIFICATION: 22-13 (Physical Organic Chemistry)  
ABSTRACT: The reaction constant  $\rho^+$  [determined from  $\sigma^+$  substituent consts. in p-RC<sub>6</sub>H<sub>4</sub>Et (I)] for the H-abstraction reaction with PhCMe<sub>2</sub>OO• was more statistically reliable than  $\rho$ , reflecting the significant contribution of polar conjugation of R with the reaction center in transition-state stabilization. The absolute magnitude of  $\rho^+$ , on the basis of current and literature evaluations, decreased in the series RC<sub>6</sub>H<sub>4</sub>Me > I > RC<sub>6</sub>H<sub>4</sub>CHMe<sub>2</sub>, reflecting the Hammond reactivity-selectivity principle.

SUPPL. TERM: abstraction hydrogen ethylbenzene deriv kinetics;  
substituent effect hydrogen abstraction ethylbenzene;  
reaction const hydrogen abstraction ethylbenzene; benzene  
alkyl reactivity selectivity

INDEX TERM: Reaction constant  
(for abstraction reaction of hydrogen from ethylbenzene  
derivs. with cumylperoxy radical)

INDEX TERM: Kinetics of abstraction reaction  
(of hydrogen, from ethylbenzene derivs. with cumylperoxy  
radical)

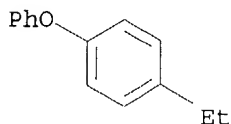
INDEX TERM: Substituent effect  
(on abstraction reaction of hydrogen from ethylbenzene  
derivs. with cumylperoxy radical)

INDEX TERM: 141-93-5, m-Diethylbenzene 937-30-4, p-Acetyethylbenzene  
1515-95-3, p-Methoxyethylbenzene 1585-07-5,  
p-Bromoethylbenzene 36207-23-5  
ROLE: PRP (Properties)  
(abstraction reaction of hydrogen of, with cumylperoxy  
radical, kinetics of)

INDEX TERM: 7175-54-4, Cumylperoxy radical  
ROLE: PRP (Properties)  
(abstraction reaction of hydrogen of, with ethylbenzene  
derivs., kinetics of)

IT 36207-23-5  
RL: PRP (Properties)  
(abstraction reaction of hydrogen of, with cumylperoxy radical,  
kinetics of)

RN 36207-23-5 HCAPLUS  
CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1989:231286 HCAPLUS  
 DOCUMENT NUMBER: 110:231286  
 ENTRY DATE: Entered STN: 25 Jun 1989  
 TITLE: Process for the preparation of 2-(substituted phenyl)propionates as pharmaceuticals or their intermediates  
 INVENTOR(S): Takahashi, Eiji; Ozaki, Kazuo; Yamada, Takao  
 PATENT ASSIGNEE(S): Maruzen Petrochemical Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 INT. PATENT CLASSIF.:  
     MAIN: C07C059-64  
     SECONDARY: B01J031-22; C07C051-14; C07C067-38; C07C069-734  
 CLASSIFICATION: 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
                   Section cross-reference(s): 1  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63290842	A2	19881128	JP 1987-125684	19870525
PRIORITY APPLN. INFO.: MARPAT 110:231286			JP 1987-125684	19870525
OTHER SOURCE(S):				

## ABSTRACT:

Title compds. R1OC6H4CHMeCO2R2 (R1 = Ph, Me; R2 = H, alkyl), e.g. phenopropylene, are prepared by dehydrogenation of R1OC6H4Et in the presence of a dehydrogenation catalyst at 400-700° and carbonylation of the resultant R1OC6H4CH:CH2 in H2O or an alc. in the presence of a Pd catalyst. 3-PhOC6H4Et and H2O at 0.5 h-1 LHSV were charged in a reactor containing tin oxide at 580°, to give 3-PhOC6H4CH:CH2 in 61.3% yield, and the product was autoclaved with Me2CHOH, PdCl2(PPh3)2, PPh3, and 35% HCl at 110° and 120 kg/cm2 CO to give total 99.8% yield of 3-PhOC6H4CHMeCO2CHMe2 and 3-PhOC6H4(CH2)2CO2CHMe2 (93.2% and 6.4% selectivity, resp.).

SUPPL. TERM: phenylpropionate prepn pharmaceutical intermediate  
 INDEX TERM: Pharmaceuticals  
               (intermediates for, phenylpropionates as)  
 INDEX TERM: Alkoxycarbonylation  
               (of styrene derivs., phenylpropionates from)  
 INDEX TERM: 1515-95-3, 4-Methoxyphenylethane 10568-38-4,  
               3-Methoxyphenylethane 36207-23-5,  
               4-Phenoxyphenylethane 78427-95-9, 3-Phenoxyphenylethane  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
               (dehydrogenation of, styrene derivative from)  
 INDEX TERM: 4973-29-9P, 4-Phenoxyphenylethylene 10568-38-4P,  
               3-Methoxyphenylethane 78427-95-9P, 3-Phenoxyphenylethane  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
               (Preparation); RACT (Reactant or reagent)  
               (preparation and alkoxy carbonylation of)  
 INDEX TERM: 637-69-4P, 4-Methoxyphenylethylene  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
               (Preparation); RACT (Reactant or reagent)  
               (preparation and alkoxy carbonylation of)  
 INDEX TERM: 113777-15-4P, Isopropyl 3-(3-methoxyphenyl)propionate  
               120824-59-1P, Isopropyl 3-(3-phenoxyphenyl)propionate  
               120824-60-4P, sec-Butyl 3-(4-phenoxyphenyl)propionate 120824-61-5P, sec-Butyl

3-(4-methoxyphenyl)propionate

ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

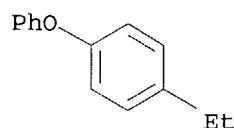
INDEX TERM: 120824-55-7P, Isopropyl 2-(3-phenoxyphenyl)propionate  
 120824-56-8P, sec-Butyl 2-(3-phenoxyphenyl)propionate  
 120824-57-9P, sec-Butyl 2-(4-methoxyphenyl)propionate  
 120824-58-0P, Isopropyl 2-(3-methoxyphenyl)propionate  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as intermediate for drugs)

IT 36207-23-5, 4-Phenoxyphenylethane

RL: RCT (Reactant); RACT (Reactant or reagent)  
(dehydrogenation of, styrene derivative from)

RN 36207-23-5 HCAPLUS

CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)

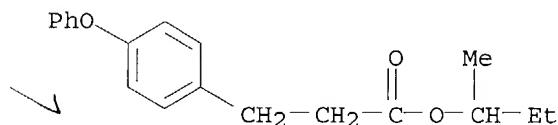


IT 120824-60-4P, sec-Butyl 3-(4-phenoxyphenyl)propionate

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 120824-60-4 HCAPLUS

CN Benzenepropanoic acid, 4-phenoxy-, 1-methylpropyl ester (9CI) (CA INDEX NAME)



L24 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:594298 HCAPLUS

DOCUMENT NUMBER: 111:194298

ENTRY DATE: Entered STN: 25 Nov 1989

TITLE: Preparation of substituted phenylpropionaldehydes as  
drug intermediates

INVENTOR(S): Takahashi, Eiji; Ozaki, Kazuo; Yamada, Takao

PATENT ASSIGNEE(S): Maruzen Petrochemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

INT. PATENT CLASSIF.:

MAIN: C07C047-277

SECONDARY: C07C045-50

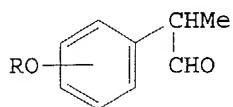
CLASSIFICATION: 25-15 (Benzene, Its Derivatives, and Condensed  
Benzenoid Compounds)

Section cross-reference(s): 1

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63290837	A2	19881128	JP 1987-125683	19870525
PRIORITY APPLN. INFO.:			JP 1987-125683	19870525
OTHER SOURCE(S):		MARPAT 111:194298		
GRAPHIC IMAGE:				



## ABSTRACT:

The title compds. I (R = Ph, Me), useful as drug intermediates, were prepared Dehydrogenation of 3-phenoxyphenylethane, followed by hydroformylation of the product in the presence of (Ph<sub>3</sub>P)<sub>3</sub>Rh(CO)H under H and CO, gave 2-(3-phenoxyphenyl)propionaldehyde with 91% selectivity and 99.1% conversion of 3-phenoxyphenylethylene.

SUPPL. TERM: phenylpropionaldehyde prepn drug intermediate; fenoprofen intermediate phenylpropionaldehyde prepn; hydroformylation phenylethylene

INDEX TERM: Hydroformylation  
(of phenylethylenes)

INDEX TERM: 17185-29-4, Hydridocarbonyltris(triphenylphosphine)rhodium  
ROLE: CAT (Catalyst use); USES (Uses)  
(catalyst, for hydroformylation of phenylethylenes)

INDEX TERM: 1515-95-3 10568-38-4, 3-Methoxyphenylethane  
**36207-23-5**, 4-Phenoxyphenylethane 78427-95-9, 3-Phenoxyphenylethane  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(dehydrogenation of)

INDEX TERM: 20401-88-1P 40138-66-7P 54954-44-8P 122801-83-6P  
ROLE: SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, in preparation of drug intermediate)

INDEX TERM: 630-08-0  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(hydroformylation, of phenylethylenes)

INDEX TERM: 29679-58-1  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(intermediates for, preparation of phenylpropionaldehydes as)

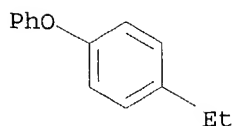
INDEX TERM: 626-20-0P 637-69-4P, 4-Methoxyphenylethylene 4973-29-9P, 4-Phenoxyphenylethylene 63444-54-2P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydroformylation of)

INDEX TERM: 5405-83-4P 59452-86-7P 59908-87-1P 80793-26-6P 123490-60-8P 123490-61-9P  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as drug intermediate)

IT **36207-23-5**, 4-Phenoxyphenylethane  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(dehydrogenation of)

RN 36207-23-5 HCAPLUS

CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



L24 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:17058 HCAPLUS

DOCUMENT NUMBER: 106:17058

ENTRY DATE: Entered STN: 24 Jan 1987

TITLE: Biotechnological preparation of optically active  $\alpha$ -arylalkanoic acids

INVENTOR(S): Cesti, Pietro; Piccardi, Paolo

PATENT ASSIGNEE(S): Montedison S.p.A., Italy

SOURCE: Eur. Pat. Appl., 11 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

INT. PATENT CLASSIF.:

MAIN: C12P007-40

SECONDARY: C12P017-14; C12P041-00

CLASSIFICATION: 16-5 (Fermentation and Bioindustrial Chemistry)

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 195717	A2	19860924	EP 1986-400558	19860317
EP 195717	A3	19890222		
EP 195717	B1	19911009		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
AT 68210	E	19911015	AT 1986-400558	19860317
US 4762793	A	19880809	US 1986-840856	19860318
JP 61239899	A2	19861025	JP 1986-61067	19860320
HU 41069	A2	19870330	HU 1986-1202	19860321
HU 197943	B	19890628		
ES 553215	A1	19870516	ES 1986-553215	19860321

PRIORITY APPLN. INFO.:

IT 1985-20036 19850322

EP 1986-400558 19860317

OTHER SOURCE(S): CASREACT 106:17058

ABSTRACT:

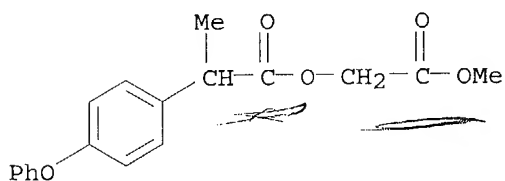
S(T) $\alpha$ -arylalkanoic acids are efficiently obtained from racemic esters by using an esterase produced by a microorganism that is capable of asym. hydrolyzing the racemic ester, i.e. capable of selectively hydrolyzing the S(t) enantiomer, in order to yield an acid substantially in the S(t) form, while leaving the ester in the R(-) form unaltered. Thus, lipase from Candida cylindracea was reacted with the ethoxycarbomethyl ester of (R,S) 2-(4-isobutylphenyl)propionic acid for 24 h at 28° to yield the S(+) acid at a conversion rate of 45% equal to 90% hydrolysis of the S(+) form.

SUPPL. TERM: arylalkanoate asym hydrolysis esterase microorganism;  
carboxylate asym hydrolysis esterase

INDEX TERM: Asymmetric synthesis and induction  
(arylalkanoic acid manufacture by, with lipase of Candida cylindracea)

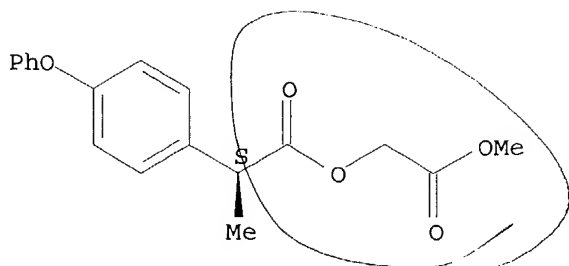
INDEX TERM: Microorganism  
(esterase of, arylalkanoic acid manufacture by asym.

hydrolysis with)  
INDEX TERM: Candida rugosa  
(lipase of, arylalkanoic acid manufacture by asym. hydrolysis with)  
INDEX TERM: Carboxylic acids, preparation  
ROLE: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)  
(aryl, manufacture of, by asym. hydrolysis with esterase of microorganisms)  
INDEX TERM: 9013-79-0  
ROLE: BIOL (Biological study)  
(arylalkanoic acid manufacture by asym. hydrolysis with, of microorganism)  
INDEX TERM: 9001-62-1, Lipase  
ROLE: BIOL (Biological study)  
(arylalkanoic acid manufacture by asym. hydrolysis with, of Candida cylindracea)  
INDEX TERM: 64622-29-3 105052-65-1 105888-62-8 105888-63-9  
105888-65-1 105888-66-2 **105888-67-3**  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(asym. hydrolysis of, to arylalkanoic acid, with lipase of microorganisms)  
INDEX TERM: 23981-80-8P 51146-56-6P 105888-60-6P 105888-64-0P  
105929-99-5P 105930-00-5P 105930-01-6P  
**105930-02-7P** 105930-03-8P 105930-04-9P  
ROLE: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)  
(manufacture of, by asym. hydrolysis with esterase of microorganisms)  
IT **105888-67-3**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(asym. hydrolysis of, to arylalkanoic acid, with lipase of microorganisms)  
RN 105888-67-3 HCAPLUS  
CN Benzeneacetic acid,  $\alpha$ -methyl-4-phenoxy-, 2-methoxy-2-oxoethyl ester  
(9CI) (CA INDEX NAME)



IT **105930-02-7P**  
RL: BMF (Bioindustrial manufacture); BIOL (Biological study); PREP (Preparation)  
(manufacture of, by asym. hydrolysis with esterase of microorganisms)  
RN 105930-02-7 HCAPLUS  
CN Benzeneacetic acid,  $\alpha$ -methyl-4-phenoxy-, 2-methoxy-2-oxoethyl ester,  
(S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1984:551531 HCAPLUS  
 DOCUMENT NUMBER: 101:151531  
 ENTRY DATE: Entered STN: 27 Oct 1984  
 TITLE: Thallium in organic synthesis. 62. A convenient synthesis of  $\alpha$ -arylsuccinic acids  
 AUTHOR(S): Taylor, Edward C.; Conley, Richard A.; Katz, Alan H.; McKillop, Alexander  
 CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, 08544, USA  
 SOURCE: Journal of Organic Chemistry (1984), 49(20), 3840-1  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 CLASSIFICATION: 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 OTHER SOURCE(S): CASREACT 101:151531

ABSTRACT:  
 $\alpha$ -Arylsuccinic acids are readily prepared by oxidative rearrangement of  $\beta$ -aroylpropionic acids (from arenes and succinic anhydride) with  $\text{Ti}(\text{NO}_3)_3 \cdot \text{HC}(\text{OMe})_3$ . Application of the same reaction to  $\beta$ -benzoylbutyric acid,  $\beta$ -benzoylvaleric acid, 1,2-dibenzoylthane and 1,4-dibenzoylbutane gives di-Me  $\alpha$ -phenylglutarate, di-Me  $\alpha$ -phenyladipate, di-Me  $\alpha, \alpha'$ -diphenylsuccinate, and di-Me  $\alpha, \alpha'$ -diphenyladipate, resp. Oxidative rearrangement of unsym. 1,2-diaroylethanes gives unsym. di-Me  $\alpha, \alpha'$ -diarylsuccinates.

SUPPL. TERM: benzoylalkanoic acid oxidative rearrangement; benzoylalkane di oxidative rearrangement; alkanolic acid benzoyl oxidative rearrangement; alkane dibenzoyl oxidative rearrangement; oxidative rearrangement dibenzoylalkane benzoylalkanoic acid; thallium nitrate oxidative rearrangement  
 INDEX TERM: Oxidation  
 (rearrangement and, of benzoylalkanoic acids and dibenzoylalkanes with thallium trinitrate and tri-Me orthoformate, diesters by)  
 INDEX TERM: Rearrangement  
 (oxidative, of benzoylalkanoic acids and dibenzoylalkanes with thallium trinitrate and tri-Me orthoformate, diesters by)  
 INDEX TERM: 5447-74-5 25333-24-8 39560-31-1 57498-54-1  
 67173-95-9 91266-23-8  
 ROLE: PROC (Process)  
 (conversion of, to enol ether)  
 INDEX TERM: 366-77-8 495-71-6 2051-95-8 3153-44-4 3375-38-0  
 4144-62-1 4619-20-9 36330-86-6 51908-41-9 89229-73-2  
 91266-20-5 91266-21-6 91266-22-7 91266-24-9  
 91266-25-0 91266-26-1  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (oxidative rearrangement of, with thallium trinitrate and

INDEX TERM: tri-Me orthoformate)  
 1496-23-7P 10436-86-9P 15463-92-0P 22248-26-6P  
 36265-44-8P 81631-72-3P **91266-19-2P**  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, by oxidative rearrangement of benzoylalkanoic  
 acid with thallium trinitrate and tri-Me orthoformate)

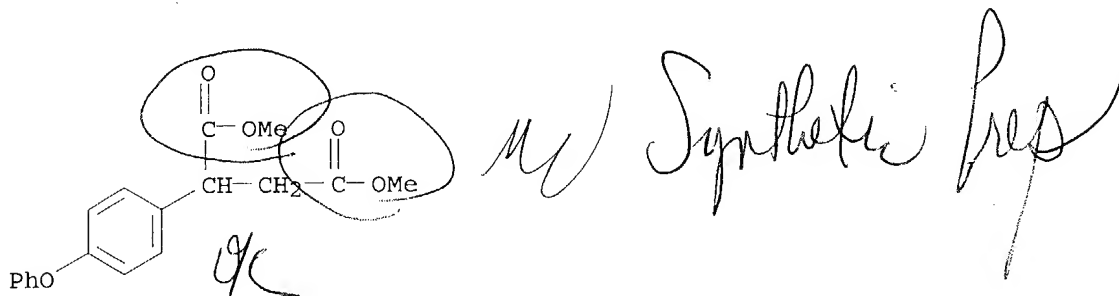
INDEX TERM: 7300-04-1P 19020-59-8P 91280-66-9P  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, by oxidative rearrangement of dibenzoylalkane  
 with thallium nitrate and tri-Me orthoformate)

INDEX TERM: 149-73-5  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (thallium trinitrate and, oxidative rearrangement of  
 benzoylalkanoic acids and dibenzoylalkanes by)

INDEX TERM: 13746-98-0  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (tri-Me orthoformate and, oxidative rearrangement of  
 benzoylalkanoic acids and dibenzoylalkanes by)

IT **91266-19-2P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, by oxidative rearrangement of benzoylalkanoic acid with  
 thallium trinitrate and tri-Me orthoformate)

RN 91266-19-2 HCAPLUS  
 CN Butanedioic acid, (4-phenoxyphenyl)-, dimethyl ester (9CI) (CA INDEX  
 NAME)



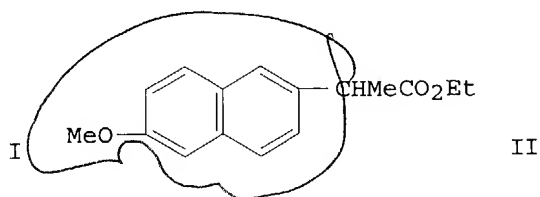
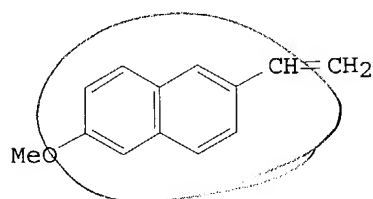
L24 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1977:467848 HCAPLUS  
 DOCUMENT NUMBER: 87:67848  
 ENTRY DATE: Entered STN: 12 May 1984  
 TITLE:  $\alpha$ -Aryl-substituted propionic acids  
 INVENTOR(S): Takeda, Makoto; Uchide, Masayuka; Iwane, Hiroshi  
 PATENT ASSIGNEE(S): Mitsubishi Petrochemical Co., Ltd., Japan  
 SOURCE: Ger. Offen., 43 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 INT. PATENT CLASSIF.: C07C069-76  
 CLASSIFICATION: 23-16 (Aliphatic Compounds)  
 Section cross-reference(s): 25, 26  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2646792	A1	19770428	DE 1976-2646792	19761016
DE 2646792	C2	19850509		
JP 52051338	A2	19770425	JP 1975-127787	19751023



JP 59035899	B4	19840831		
JP 60045171	B4	19851008	JP 1976-91523	19760731
GB 1565235	A	19800416	GB 1976-43221	19761018
FR 2328689	A1	19770520	FR 1976-32143	19761025
FR 2328689	B1	19830121		
US 4329507	A	19820511	US 1980-111978	19800114
PRIORITY APPLN. INFO.:			JP 1975-127787	19751023
			JP 1976-91523	19760731
			US 1976-734592	19761021
			US 1978-909643	19780525

OTHER SOURCE(S): CASREACT 87:67848  
 GRAPHIC IMAGE:



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## ABSTRACT:

Alkoxy carbonylation by alcs. and CO and carboxylation by H<sub>2</sub>O and CO of vinylarenes were catalyzed by Pd complexes. Thus, I in EtOH containing (Ph<sub>3</sub>P)<sub>2</sub>PdCl<sub>2</sub>, BF<sub>3</sub>·Et<sub>2</sub>O, and Ph<sub>2</sub>NNO was autoclaved with CO to give 69% II.

SUPPL. TERM: alkoxy carbonylation vinylarene catalyst; carboxylation vinylarene catalyst; propionic acid aryl

INDEX TERM: Alkoxy carbonylation catalysts  
(palladium complexes, for vinylarenes)

INDEX TERM: 5338-96-5  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(Grignard reaction of)

INDEX TERM: 391-08-2 716-89-2 3139-85-3 4973-29-9 10473-10-6  
30215-52-2 54314-33-9 63444-51-9 63444-52-0  
63444-53-1 63444-54-2 63444-55-3 63444-56-4  
63444-57-5  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(alkoxy carbonylation of)

INDEX TERM: 109-63-7 603-35-0, uses and miscellaneous 7647-10-1  
13965-03-2 14977-08-3  
ROLE: CAT (Catalyst use); USES (Uses)  
(catalyst, for alkoxy carbonylation of vinylarenes)

INDEX TERM: 62049-65-4  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(dehydrochlorination of)

INDEX TERM: 5002-42-6 42771-85-7  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(hydride reduction of)

INDEX TERM: 40150-92-3P 56430-69-4P 63444-59-7P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and dehydration of)

INDEX TERM: 56430-44-5P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and dehydrohalogenation of)

INDEX TERM: 37961-57-2P 41283-72-1P 61001-75-0P  
61566-34-5P 63444-58-6P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)

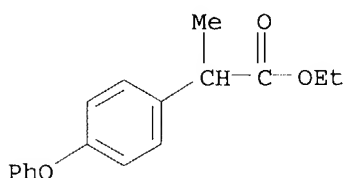
INDEX TERM: 3585-53-3P 5005-84-5P 6908-47-0P 15687-27-1P  
17692-38-5P 22410-97-5P 23981-80-8P 29679-58-1P  
36141-62-5P 36950-96-6P 41604-03-9P 51106-57-1P  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 61001-75-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)

RN 61001-75-0 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -methyl-4-phenoxy-, ethyl ester (9CI) (CA INDEX NAME)



L24 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:592403 HCAPLUS

DOCUMENT NUMBER: 85:192403

ENTRY DATE: Entered STN: 12 May 1984

TITLE: Phenoxyphenylbutyric acid derivatives

INVENTOR(S): Gante, Joachim; Kurmeier, Hans A.; Schacht, Erich; Mehrhof, Werner; Wild, Albrecht

PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Fed. Rep. Ger.

SOURCE: Ger. Offen., 51 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

INT. PATENT CLASSIF.: ~~C07C069~~-76

CLASSIFICATION: 25-18 (Noncondensed Aromatic Compounds)

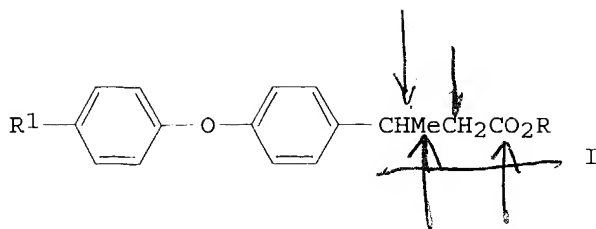
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2509891	A1	19760923	DE 1975-2509891	19750307
SE 7602744	A	19760908	SE 1976-2744	19760227
AU 7611555	A1	19770908	AU 1976-11555	19760302
AU 497104	B2	19781130		
BE 839211	A2	19760906	BE 1976-7000789	19760304
FR 2302731	A1	19761001	FR 1976-6130	19760304
DK 7600979	A	19760908	DK 1976-979	19760305
NL 7602341	A	19760909	NL 1976-2341	19760305
ZA 7601340	A	19770223	ZA 1976-1340	19760305
ES 445793	A1	19770901	ES 1976-445793	19760305
GB 1494462	A	19771207	GB 1976-8980	19760305
AT 7601624	A	19790515	AT 1976-1624	19760305
JP 51125348	A2	19761101	JP 1976-25990	19760308
			DE 1975-2509891	19750307

PRIORITY APPLN. INFO.:

GRAPHIC IMAGE:



~~XX~~ *Formula*

## ABSTRACT:

The title compds. (I; R = H, Me, Et, Pr, Bu, tert-Bu, Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>, Me<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>; R<sub>1</sub> = H, Br, Cl, F), useful as analgesics and antipyretics, are prepared by a variety of standard procedures. Thus, reduction and hydrolysis of 4-(4-ClC<sub>6</sub>H<sub>4</sub>O)C<sub>6</sub>H<sub>4</sub>CMe(OH)CH<sub>2</sub>CO<sub>2</sub>Et with 67% aqueous HI in AcOH 1 hr at 150° gives I (R = H, R<sub>1</sub> = Cl).

SUPPL. TERM: phenoxyphenylbutyrate analgesic antipyretic; butyrate  
halophenoxyphenyl analgesic antipyretic

INDEX TERM: Analgesics  
Antipyretics  
([(halophenoxy)phenyl]butyrate acid derivs.)

INDEX TERM: 55102-99-3  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(Grignard reaction with K 3-iodobutyrate)

INDEX TERM: 61001-87-4 61001-88-5  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(Grignard reaction with carbon dioxide)

INDEX TERM: 78-09-1 124-38-9, reactions 541-41-3 61001-86-3  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(Grignard reaction with halophenyl ethers)

INDEX TERM: **61001-75-0**  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(chlorination of)

INDEX TERM: 61001-98-7  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(deamination and fluoroamination of)

INDEX TERM: 61001-97-6  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(deamination of)

INDEX TERM: 61001-90-9 61001-91-0  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(decarboxylation of)

INDEX TERM: 60467-98-3 61001-74-9  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(hydrogenation and hydrolysis of)

INDEX TERM: 61001-76-1 61024-36-0  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(hydrogenation of)

INDEX TERM: 61001-89-6  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis and decarboxylation of)

INDEX TERM: 58727-42-7 58727-45-0  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis and reduction of)

INDEX TERM: 61001-78-3 61001-79-4 61001-80-7 61001-81-8  
61001-82-9  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis of)

INDEX TERM: 58727-63-2 61001-94-3  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(oxidation of)

INDEX TERM: 61001-57-8P 61001-61-4P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and esterification of)

INDEX TERM: 61001-58-9P 61001-64-7P 61001-65-8P 61001-66-9P  
61001-67-0P 61001-71-6P 61001-72-7P 61001-73-8P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)

INDEX TERM: 61001-59-0P 61001-60-3P 61001-63-6P 61001-68-1P  
61001-70-5P  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

INDEX TERM: 1099-45-2  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with 4-(1-bromoethyl)-4'-fluorodiphenyl ether)

INDEX TERM: 61024-35-9  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with carbon monoxide)

INDEX TERM: 1951-12-8 7425-49-2  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with chlorophenyl phenyl ether)

INDEX TERM: 61001-95-4  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with diethylamine)

INDEX TERM: 352-34-1  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with disodium 3-(4-hydroxyphenyl)butyrate)

INDEX TERM: 61001-77-2  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with ethyl [triphenylphosphoranylidene]acetate)

INDEX TERM: 61001-83-0 61001-84-1  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with ethyl bromobutyrate)

INDEX TERM: 61024-34-8  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with fluoroiodobenzene)

INDEX TERM: 61001-93-2  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with formic acid and with nickel carbonyl)

INDEX TERM: 7005-72-3  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with halobutyrate)

INDEX TERM: 13463-39-3  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with halophenyl ethers)

INDEX TERM: 61001-92-1  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with nickel carbonyl)

INDEX TERM: 100-35-6 107-99-3  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with sodium [(chlorophenoxy)phenyl]butyrate)

INDEX TERM: 61001-96-5  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with sodium fluorophenolate)

INDEX TERM: 61001-85-2  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with tert-butyl alc. and propanol)

INDEX TERM: 371-35-7  
ROLE: RCT (Reactant); RACT (Reactant or reagent)

INDEX TERM: (reaction with sodium (iodophenyl)butyrate)  
64-18-6, reactions  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(with 4-chlorophenyl 4-(2-propenyl)phenyl ether)

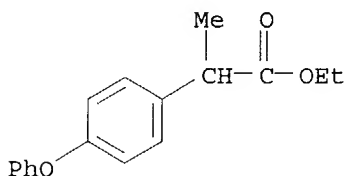
INDEX TERM: 630-08-0, reactions  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(with [(chlorophenoxy)phenyl]propanol)

INDEX TERM: 109-89-7, reactions  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(with chloroethyl [(chlorophenoxy)phenyl]butyrate)

IT 61001-75-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(chlorination of)

RN 61001-75-0 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -methyl-4-phenoxy-, ethyl ester (9CI) (CA  
INDEX NAME)



L24 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1972:144751 HCAPLUS

DOCUMENT NUMBER: 76:144751

ENTRY DATE: Entered STN: 12 May 1984

TITLE: Effect of introducing ethyl radical to benzene derivatives on their odorant properties

AUTHOR(S): Wizner, Iwonna

CORPORATE SOURCE: \* Inst. Chem. Przem., Warsaw, Pol.

SOURCE: Tluszcze, Srodki Piorace, Kosmetyki (1971), 15(5), 20-30  
CODEN: TSPKBZ; ISSN: 0372-1795

DOCUMENT TYPE: Journal

LANGUAGE: Polish

CLASSIFICATION: 62 (Essential Oils and Cosmetics)

ABSTRACT: The effects of Et groups on odorant properties was studied in large number of esters, alcs., aldehydes, and ketones, as well as in p-ethyldiphenylmethane (I) and p-ethyldiphenyl ether. The most interesting scent was found in p-ethylacetophenone, I, Me p-ethylbenzoate, and p-ethylphenyl- $\beta$ -butyl alc. Many of the compds. synthesized are not found in literature.

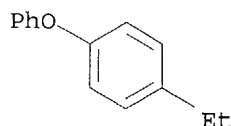
SUPPL. TERM: ethyl groups odorant; ester odorant ethyl effect; alc odorant ethyl effect; aldehyde odorant ethyl effect; ketone odorant ethyl effect

INDEX TERM: Molecular structure-property relationship  
(benzene ethyl derivs., odors)

INDEX TERM: Alcohols, properties  
Aldehydes, properties  
Esters, properties  
Ketones, properties  
ROLE: PRP (Properties)  
(odors of, ethyl radicals in relation to)

INDEX TERM: Odor and Odorous substances

(of benzene ethyl derivs.)  
 INDEX TERM: 768-59-2 4748-78-1 14062-20-5 22545-13-7 36207-03-1  
 36207-04-2 36207-05-3 36207-06-4 36207-07-5  
 36207-08-6 36207-09-7 36207-10-0 36207-13-3  
 36207-14-4 36207-15-5 36207-16-6 36207-18-8  
 36207-19-9 36305-78-9  
 ROLE: PRP (Properties)  
 (odor of)  
 INDEX TERM: 620-85-9 937-30-4 7364-20-7 36207-23-5  
 ROLE: PRP (Properties)  
 (odors of)  
 INDEX TERM: 36207-25-7P  
 ROLE: PREP (Preparation)  
 (preparation of)  
 IT 36207-23-5  
 RL: PRP (Properties)  
 (odors of)  
 RN 36207-23-5 HCAPLUS  
 CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 13-

YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):yn

YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):n

=> d ibib abs hitstr 14-

YOU HAVE REQUESTED DATA FROM 2 ANSWERS - CONTINUE? Y/(N):y

L24 ANSWER 14 OF 15 USPATFULL on STN

ACCESSION NUMBER: 88:50260 USPATFULL

TITLE: Process for the biotechnological preparation of optically active alpha-arylalkanoic acids

INVENTOR(S): Cesti, Pietro, Novara, Italy

Piccardi, Paolo, Milan, Italy

PATENT ASSIGNEE(S): Montedison S.p.A., Milan, Italy (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4762793		19880809
APPLICATION INFO.:	US 1986-840856		19860318 (6)

	NUMBER	DATE
PRIORITY INFORMATION:	IT 1985-20036	19850322
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Rosen, Sam	
LEGAL REPRESENTATIVE:	Morgan & Finnegan	
NUMBER OF CLAIMS:	5	
EXEMPLARY CLAIM:	1	
LINE COUNT:	301	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB There is described the preparation of S(+) alpha-aryl-alkanoic acids by means of the reaction of a racemic ester(R,S) of the formula: ##STR1## wherein: R is a group selected from the group consisting of --C.tbd.CH, a --CH.dbd.CH.sub.2, --CN; --COCH.sub.3, --COO alkyl C.sub.1 C.sub.4 and --CH.sub.2 --O alkyl C.sub.1 -C4 group, Ar is a group selected from the group consisting of an aryl group and an aryl substituted or condensed with other groups, in particular a group selected from the group consisting of groups of the formula: ##STR2## wherein: R' is selected from the group consisting of C.sub.1 -C.sub.8 linear or branch of chain alkyl, C.sub.1 -C.sub.4 alkenyl, alkoxy, phenyl, phenoxy, tenoyl and heterocyclic;

R" is selected from the group consisting of hydrogen or halogen;

R''' is a C.sub.1 -C.sub.4 alkyl,

with an esterase, produced by microorganisms capable of selectively hydrolyzing the S(+) form of said racemic ester and by successively separating the S(+) acid from the unreacted ester.

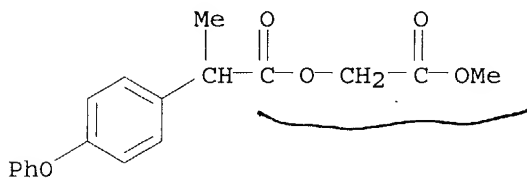
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 105888-67-3

(asym. hydrolysis of, to arylalkanoic acid, with lipase of microorganisms)

RN 105888-67-3 USPATFULL

CN Benzeneacetic acid, alpha-methyl-4-phenoxy-, 2-methoxy-2-oxoethyl ester (9CI) (CA INDEX NAME)



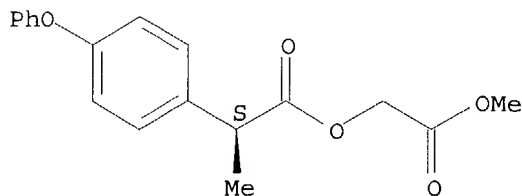
IT 105930-02-7P

(manufacture of, by asym. hydrolysis with esterase of microorganisms)

RN 105930-02-7 USPATFULL

CN Benzeneacetic acid, alpha-methyl-4-phenoxy-, 2-methoxy-2-oxoethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 15 OF 15 USPATFULL on STN

ACCESSION NUMBER: 82:22897 USPATFULL

TITLE: Substituted aryl ethylenes

INVENTOR(S): Takeda, Makoto, Amimachi, Japan

PATENT ASSIGNEE(S): Uchide, Masayuki, Amimachi, Japan  
Iwane, Hiroshi, Amimachi, Japan  
Mitsubishi Petrochemical Co., Ltd., Tokyo, Japan  
(non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4329507		19820511
APPLICATION INFO.:	US 1980-111978		19800114 (6)
RELATED APPLN. INFO.:	Division of Ser. No. US 1978-909643, filed on 25 May 1978, now abandoned which is a division of Ser. No. US 1976-734592, filed on 21 Oct 1976, now abandoned		

	NUMBER	DATE
PRIORITY INFORMATION:	JP 1975-127787	19751023
	JP 1976-91523	19760731
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Chan, Nicky	
ASSISTANT EXAMINER:	Reamer, J. H.	
LEGAL REPRESENTATIVE:	Burns, Robert E., Lobato, Emmanuel J., Adams, Bruce L.	
NUMBER OF CLAIMS:	3	
EXEMPLARY CLAIM:	1,2,3	
LINE COUNT:	317	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB New substituted aryl ethylenes are disclosed which are produced by dehydration of the corresponding  $\alpha$ - or  $\beta$ -(substituted aryl)ethyl alcohols or by dehydrohalogenation of the corresponding  $\alpha$ - or  $\beta$ -(substituted aryl)ethyl halides.

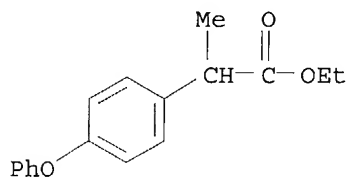
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 61001-75-0P

(preparation and hydrolysis of)

RN 61001-75-0 USPATFULL

CN Benzeneacetic acid,  $\alpha$ -methyl-4-phenoxy-, ethyl ester (9CI) (CA INDEX NAME)



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